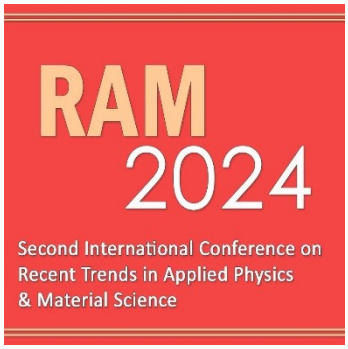
Abstract Book of
2nd International Conference on Recent Trends in Applied Physics & Material Science

RAM 2024
November 15-16, 2024



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Preface: RAM 2024

It is with immense pleasure that we welcome you all to the *International Conference on Recent Trends in Applied Physics and Material Science 'RAM 2024'*. This year's conference, held in hybrid mode, reflects our commitment to fostering collaboration, innovation, and knowledge-sharing across borders. With over 500 participants joining us from various parts of the globe, 'RAM 2024' is set to be a vibrant platform for the exchange of cutting-edge research and emerging ideas in the fields of applied physics and material science.

The purpose of 'RAM 2024' is to bring together researchers, industry experts, academicians, and students to engage in discussions on the latest advancements in applied physics and material science domains. As science and technology continue to evolve rapidly, the contributions made here will play a vital role in addressing contemporary challenges and pushing the boundaries of knowledge. This conference not only offers a forum for the presentation of groundbreaking research but also provide opportunities for meaningful dialogue, networking, and collaboration, which are crucial to the advancement of scientific discovery.

From theoretical physics to practical applications in material science, the abstracts highlight the depth and breadth of work that our participants have contributed. Each abstract represents months or even years of dedicated effort and exemplifies the spirit of inquiry that drives scientific progress. This abstract book serves as a comprehensive guide to the diverse range of research topics and presentations that will be showcased in 'RAM 2024'.

We are grateful to all the presenters, attendees, and supporters who have made 'RAM 2024' possible. Special thanks to the organizing committee, sponsors, and volunteers whose tireless efforts have ensured the success of this event. We hope that the discussions sparked during the conference will lead to fruitful collaborations and inspire further research in the coming years.

Thank you for your participation, and we wish you an intellectually stimulating and rewarding experience at 'RAM 2024'.

Warm regards,

November 14, 2023

Sudhir Bhardwaj
Manoj Singh Shekhawat
Bhuvneshwer Suthar
(Editors)

Message from the Vice-Chancellor

It is a matter of immense pride and pleasure to welcome all esteemed participants, delegates, and distinguished guests to the Recent Trends in Applied Physics and Material Science (RAM 2024) conference, organized under the aegis of Bikaner Technical University. As the Chief Patron of this prestigious event, I am deeply honored to witness the confluence of brilliant minds from across the globe, gathered to exchange groundbreaking ideas and innovative research in applied physics and material science.

RAM 2024 stands as a testament to our commitment to advancing scientific knowledge and fostering an environment conducive to interdisciplinary collaboration. In a world marked by rapid technological and scientific advancements, this conference serves as a platform for scholars, researchers, and practitioners to share insights, discuss challenges, and explore novel solutions to some of the most pressing issues in material science and its allied fields.

I extend my sincere gratitude to the organizing committee for their dedication and tireless efforts in bringing this conference to fruition. I also congratulate all participants for their contributions to the knowledge pool and wish everyone an enlightening and enriching experience at RAM 2024. May this conference not only inspire innovative research but also pave the way for future collaborations that drive progress in science and technology.

With warm regards,

[Prof. Ajay Kumar Sharma]
Vice-Chancellor, Bikaner Technical University
Chief Patron, RAM 2024

Message from the Principal

I am delighted to extend a warm welcome to all participants of the Recent Trends in Applied Physics and Material Science (RAM 2024) conference. This event marks a significant opportunity for scholars, researchers, and professionals to engage with the latest advancements and emerging trends in applied physics and material science.

At Bikaner Technical University, we take pride in fostering an academic environment that encourages collaboration, innovation, and critical thinking. RAM 2024 reflects our commitment to supporting scientific research and connecting minds across disciplines to drive progress. The insights and ideas exchanged here will not only enrich our understanding but also inspire meaningful applications that can benefit society at large.

I congratulate the organizing committee for their dedication and meticulous planning, which have made this conference possible. To all the presenters and participants, I extend my best wishes for a productive and inspiring experience. May RAM 2024 open new avenues for discovery and collaboration that will continue to impact the field of material science for years to come.

With best regards,

[Dr. Yadu Nath Singh]
Principal, Bikaner Technical University
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Programme Schedule

of 2nd International Conference on Recent Trends in Applied Physics & Material Science (RAM 2024)

Day 1 – Friday, 15 November, 2024

8:00 AM - 9:00 AM	Registration & Breakfast
9.00 AM - 9:30 AM	Inaugural Ceremony
9:30 AM - 11:00 AM	Invited Session - I
	Session Chair: **Prof. R. R. Deshmukh**, Institute of Chemical Technology, Matunga, Mumbai
	Session Co-Chair: **Prof. M.D. Sharma**, Department of Physics, Govt. Dungar College Bikaner
	Invited Lecture -1: **Prof. Nand Lal Singh**, Professor, Netaji Subhas University of Technology, New Delhi
	Invited Lecture -2: **Prof. D.K. Dwivedi**, Department of Physics & Material Science, MMMUT, Gorkhapur
11:00 AM - 11:30 AM	High Tea
11:30 AM - 01:00 PM	Invited Session-II
	Session Chair: **Prof. Nand Lal Singh**, Professor, Netaji Subhas University of Technology, New Delhi
	Session Co-Chair: **Dr. Ravindra Mangal**, Ex. VC. Global National University & Principal Govt. College, Nokha
	Invited Lecture -3: **Prof. Manoj Kumar Sharma**, University of Lucknow, Lucknow
	Invited Lecture -4: **Dr. Rajesh Kumar**, IIT Roorkee
	Invited Lecture -5: **Prof. Anami Bhargava**, Department of Physics, Govt. Dungar College, Bikaner
1:00 PM -2:00 PM	Lunch
2:00 PM -4:00 PM	Poster Session –I (offline) **(A to G - All)**
	Parallel Oral Session I (online)
	I-A (A1-0002 to A1-0037)
	I-B (A1-0038 to A1-0069)
	I-C (A1-0070 to A1-0101)

		I-D	**(A1-0102 to A1-0132)**
		I-E	**(A1-0133 to A2-0012)**
		I-F	**(A2-0013 to B2-0010)**
4:00 PM - 4:15 PM	**Tea Break**		
4:15 PM - 6:30 PM	**Oral Session (Offline)**		
	Session Chair:	**Dr. Rajesh Kumar, IIT Roorkee**	
	Session Co-Chair:	**Dr. Amit Sharma, DRDO, Jodhpur**	
	Parallel Oral Session II (Online)		
		II-A	**(B2-0011 to D2-0007)**
		II-B	**(E1-0003 to G1-0011)**
		II-C	**(G1-0012 to H1-0006)**
		II-D	**(H1-0007 to I1-0017)**
6:45 PM - 8:00 PM	**Cultural Program**		
8:00 PM Onwards	**Dinner**		

Day 2 – Saturday, 16th November, 2024

8:00 AM - 8:30 AM Morning Breakfast

8:30 AM - 10:30 AM Invited Session-III

Session Chair: **Prof. Vivek Kumar Gupta**, Department of Physics, University of Jammu, Jammu

Session Co-Chair: **Prof. A. K. Nagar**, Govt. Dungar College, Bikaner

Invited Lecture -6: **Prof. Arun Bansil**, Northeastern University, Boston, USA

Invited Lecture -7: **Prof. Pawan Kumar Kularia**, Department of Physics, Jawaharlal Nehru University, New Delhi

Invited Lecture -8: **Dr. Vinod Singh**, Delhi Technological University, New Delhi

Invited Lecture -9: **Dr. Amit Kumar** DRDO, Jodhpur

10:30 AM - 11:00 AM High Tea

11:00 AM – 1:00 PM Poster Session-II (H to W - All)

Parallel Oral Session III (online)

III-A (I1-0018 to J1-0002)
III-B (J2-0001 to L1-0008)
III-C (L1-0012 to N1-All)
III-D (O1-All and O2-All)
III-E (P1-All to S1-All)
III-F (T1-All to Z2-All)

1:00 PM-2:00 PM Lunch

2:00 PM-3:00 PM Invited Session-IV

Session Chair: **Prof. Anami Bhargava**, Govt. Dungar College, Bikaner

Session Co-Chair: **Prof. Smita Sharma**, Govt. Dungar College Bikaner

Invited Lecture-10: **Prof. R. R. Deshmukh**, Institute of Chemical Technology, Matunga, Mumbai

Invited Lecture-11: **Prof. Vivek Kumar Gupta**, Department of Physics, University of Jammu, Jammu

3:15 PM - 4:00 PM Valedictory Session

4:00 PM Tea

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IT-0001

Effect of Swift Heavy Ion Irradiation on Materials Modification and Their Applications

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Abstract

The polymeric films were synthesized using the solution casting method by incorporating the different concentrations (ie. 5,10 and 15%) of metal nanoparticles (Ni, Cu, Ag) in insulating PMMA/PS polymer matricesThese films were irradiated with swift heavy ions at different fluences. The changes in structural, optical, thermal, dielectric and magnetic properties were studied by using different characterization techniques such as XRD, UV-Vis, FTIR, DSC, etc. The results of investigations and applications will be discussed.

Materials for applications in harsh conditions, such as nuclear reactors or the immobilization of radioactive waste, require extremely strong radiation damage resistance, including resistance to volume swelling or amorphization. Here, we shall focus specifically on oxides that resemble the crystal structure of fluorite. In particular, the structural changes caused by ion irradiation, such as lattice enlargement, amorphization, and phase change from pyrochlore to fluorite, have been researched for potential applications in harsh environments. Pyrochlore oxides, a class of complex materials with a general formula $A_2B_2O_7$, have garnered significant attention due to their exceptional radiation tolerance properties for use in hostile environments, i.e., radioactive waste immobilization and nuclear reactors. We will discuss the structural changes such as lattice expansion, amorphization, and phase transformation from pyrochlore to fluorite for possible potential uses in harsh environments engendered by 1 MeV Xe^{2+} and 500 KeV Kr^{2+} ions irradiation of the pyrochlore oxides of $La_2Zr_2O_7$.

IT-0002

Optical Biosensors Using Photonic Crystals for Medical Applications

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Abstract

Photonic crystals (PCs) are artificially created microscale or nanoscale optical structures with a periodic arrangement of dielectrics with high and low refractive indices. A forbidden band, known as a photonic bandgap (PBG), is generated for a certain wavelength region due to such periodicity of the dielectric or refractive index. In a conventional 1-D PC, adding a new layer or removing one layer works as an optical cavity that introduce a defect mode at the resonant wavelength into the PBG. The geometrical characteristics of the defect layer, such as thickness and refractive index, can be tuned to affect the defect mode along with angle of incidence and number of layers on either side of defect layer. These 1-D PCs with defect layer have a wide range of possible applications, including optical filters, optical switches, tunable filters, temperature sensor, pressure sensor, optical biosensor, demultiplexers and so on. In the present work, we shall present our recent studies on optical biosensor applications of 1-D PC structure that attract the focus of research community due to their ultra-fast response, compact size and very precise result. The earliest indicator of any disease is testing of blood, stool and urine sample, whose refractive index characterization is interesting for a pathological analysis and treatment. The optical sensor parameters as sensitivity, quality factor (QF), figure of merit (FOM) and detection limit (DL) are investigated for all cases of symmetric and asymmetric structures. In the reported studies, the materials, structural changes geometrical changes, fluid density changes and concentration changes with incident wavelength range to account for enhance optical sensor parameters. The results and conclusions are presented primarily for blood samples for malaria diagnosis, tuberculosis, haemoglobin and sucrose concentration as well as for waterborne polio virus and bacterial detection.

IT-0003

Gas Phase Synthesis of Size Selected Pd and Pd-C Nanoparticles and their Gas Sensing Application

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Abstract

Size selected nanoparticles are grown by the integrated gas phase synthesis method. The core size and shell thickness in core-shell nanoparticles are independently controlled. The effect of different parameters such as spark frequency, carrier gas flow rate and sintering temperature on the growth of nanoparticles has been studied.
Hydrogen gas sensing response of Pd-C core-shell nanoparticles having a fixed core size and different shell thickness has been investigated and the effect of carbon shell around size selected Pd nanoparticles on hydrogen sensing has been studied. It is observed that Pd-C nanoparticle sensor shows higher sensitivity and faster response/ recovery in comparison to that of Pd nanoparticle samples and these parameters further improve with increase in shell thickness. Further, it has been observed that Pd-C nanoparticles exhibit H_2 sensitivity at room temperature in contrast to Pd nanoparticles which respond only at higher temperatures.

Keywords: Gas phase synthesis, Size selected nanoparticles, H_2 sensors

A1-0002

Preparation and Characterization of Nanoparticles of Fe^{3+} substituted by chromium Doping in Copper Ferrite

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Abstract

Ferrites are ceramic like material having magnetic properties which are being utilized for several applications. Nano ferrites $CuCr_xFe_{2-x}O_4$ (x= 0.2,0.4 ,0.6,0.8) were synthesized by Sol Gel Method with nitrates of Cu, Cr, Fe and citric acid. The structural characterization of these samples was done using the X- ray diffraction method (XRD). XRD patterns confirmed a well-defined single-phase cubic spinel structure and were reconfirmed by Rietveld's refinement of these XRD patterns. It has been found that as the amount of dopant (Cr) increases, size of the nano particles decreased. The morphology of sample was analyzed using FESEM.

Keywords: XRD, Rietveld refinement, FESEM.

A1-0003

Eco-Friendly Synthesis, Structural Analysis, and Antibacterial Evaluation of Pure and Cadmium-Doped Barium Oxide

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Abstract

Doped nanostructured materials have attracted considerable interest due to their enhanced structural, chemical, and physical properties compared to their undoped counterparts [1]. This study presents an eco-friendly approach for the synthesis of pure and cadmium-doped barium oxide (BaO) nanoparticles using *Pterocarpus santalinus* (sandalwood bark) extract [2]. The synthesized nanoparticles were characterized through X-ray diffraction (XRD), scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM-EDX), and their antibacterial properties were assessed against *Bacillus subtilis* (Gram-positive) and *Escherichia coli* (Gram-negative) bacteria [3]. XRD analysis confirmed that the BaO nanoparticles have a tetragonal structure, with crystallite sizes of 14.85 nm for pure BaO and 16.41 nm for Cd-doped BaO [1]. SEM images revealed that pure BaO nanoparticles are uniformly dispersed, porous, and flower-like, whereas Cd-doped BaO particles exhibited aggregation and irregular shapes [2]. Antibacterial testing indicated that both pure and Cd-doped BaO nanoparticles demonstrate significant antibacterial activity, highlighting their potential as effective antibacterial agents in the food and medical industries [3]. This study underscores the potential of green synthesis methods in developing advanced nanomaterials with practical applications.

Keywords: Cadmium-doped Barium Oxide, Eco-friendly Synthesis, Antibacterial Nanoparticles

A1-0004

Electrical Properties of Natural Fibres and Filled Polymeric Nano Composites

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Abstract

Polymeric materials are widely used by electrical insulation design engineers like immense dielectric characteristics, high strength to weight ratio, and ease of moulding and have their many uses. However, it has shown out that there are significant barriers to the widespread use of these materials, including charge buildup at high DC fields, poor discharge resistance, low thermal conductivity, a limited operating temperature range, and insufficient stiffness. Innovative dielectric materials with improved functions are crucial to the dependability of today's electrical power systems. The concept known as polymer nanocomposites is intended to offer a workable answer to the previously listed difficulties. Polymreic based nano composites are created by evenly dispersing a small amount of fillers that are nanoscale in size into a polymer matrix. This research is motivated in order to utilise polymeric natral fibre and nano filler filled materials in electrical appliances

A1-0006

Amalgamation of Discotic Liquid Crystal with Plasmonic Nanoparticles

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Abstract

Dispersion of colloidal gold nanoparticles (GNPs) in triphenylene-based discotic liquid crystal (DLC) namely 2,3,6,7,10,11- hexabutyloxytryphenylene (HAT4) possessing plastic columnar phase (Col_p) phase, has been studied by differential scanning calorimetry, polarized light microscopy, UV-Vis absorption spectroscopy, X-ray diffraction and dielectric spectroscopy. GNPs have been dispersed in three different concentrations in pure HAT4 viz 0.2, 0.6 and 1.2 wt%. It has been observed that with the increase of GNPs concentration, the Col_{hp}-Isotropic (Iso) transition temperature decreases substantially but the crystal (Cr)-Col_{hp} transition temperature does not change significantly. Electrical conductivity increases at least by five orders of magnitudes for the highest concentration of GNPs (1.2 wt%) as compared to the pure material i.e HAT4. Observed results suggest that although extremely low concentrations of GNPs are not very useful but moderate concentration is highly useful in increasing conductivity of the Col_{hp} phase and also to implant surface plasmon resonance. These results may be exploited to enhance efficiency of electro-optical devices by using HAT4-GNPs composites.

Keywords: discotic liquid crystals; columnar plastic phase; DLC-nano composites; dielectric properties; homeotropic alignment; surface plasmon resonance.

A1-0008

Synthesis and Characterization of Nanoparticles ofAluminum Doped Zinc Ferrite

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Abstract

The nano ferrite $ZnAl_xFe_{2-x}O_4$ (x=0.2,0.4,0.6,0.8) discussed in present worksynthesized using auto combustion sol gel method with nitrate of Zn, Al, Fe andcitric acid. The surface morphology of the sample was analysed using FESEM. The structural characterization of these samples was done using the X-raydiffraction method (XRD). XRD patterns confirmed a well-defined single-phasecubic spinel structure and were reconfirmed by Rietveld's refinement of these XRD patterns. The particle size of the samples showed a consistent decreasing trend with aluminum doping has been confirmed by XRD analysis.

Keywords: XRD, Rietveld refinement, FESEM.

A1-0009

MoS_2: A Reliable Material for Supercapacitor Applications

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Abstract

The ever- growing demand to deduce the gap between power and energy densitydelivered by the different energy storage devices like battery, fuel cell and supercapacitor is driving the research to look for novel electrode materials. With the increase of population, the demand of energy is continuously increasing. For this, it is a very challenging task to develop a highly effective, environment friendly, sustainable energy storage devices. Among various energystorage devices supercapacitor got special attention because the gap between battery and conventional capacitor can be fulfilled by it; which results in high power density. There are manyreported materials with high specific capacitance, but now a day, MoS_2 attains high attention dueto its high surface area, various oxidation state and ecofriendly nature. In present work, MoS_2 was synthesized by hydrothermal method which shows a highly porous flower like structure. Further, MoS_2 powder was used to fabricate the supercapacitor electrodes to investigate the electrochemical behavior using cyclic voltammetry (CV) and galvanic charge discharge (GCD) at different scan rate (5, 10, 20, 30, 50 mVs-1) and current density (0.5,1, 1.5, 2 Ag^{-1}), respectively. As a result, fabricated electrode delivered good specific capacitance (403 Fg^{-1} at 5mVs^{-1}) and outstanding cycling stability (97% up to 2000 cycles).

A1-0010

Investigation of the blue shift phenomena and dielectric behaviour with the concentration of Cobalt doped in ZnS nano-particles

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Abstract

The study involved synthesizing undoped Zinc Sulphide (ZnS) nanoparticles (NPs) and Cobalt (Co) doped ZnS NPs with varying Co concentrations. Ethylenediamine (EDA) was used as a capping agent during the hydrothermal synthesis. The investigation focused on analyzing the structural, optical, molecular, and electrical properties influenced by the Co doping. X-ray diffraction (XRD) patterns indicated crystalline nature and showed intense peaks consistent with the primary cubic phase of zinc blend. Notably, no peaks corresponding to the doped material Co were observed, indicating successful incorporation of Co ions into the host ZnS without significantly altering the original crystal structure. Additionally, a weak signature of ZnS's hexagonal phase was detected. The UV-Visible spectra revealed that the optical band gap energy varied with Cobalt concentration, confirming a quantum confinement process and a blue shift phenomena. FTIR spectra showed that the position of ZnS characteristic frequency bands remained unchanged with doping, indicating successful substitution of Zn with Co. Photo luminance (PL) spectra demonstrateda noticeable response in PL intensity with varying Co concentration. The Scanning Electron Microscope (SEM) images and Energy Dispersive X-Ray (EDX) spectra confirmed agglomerated NPs with nearly spherical shapes and stoichiometric elemental compositions. Furthermore, the measured AC conductivity values increased with higher dopant concentrations at a higher frequency range, suggesting potential applications in high-frequency regimes. Consequently, the study suggests that Co doped ZnS materials hold promise for applications in spintronics and photo luminescent devices.

Keywords: Cobalt-doped ZnS, Photo luminance, Band-gap, Fourier Transform Infrared (FTIR), AC conductivity.

A1-0012

Preparation and Characterization of Nanostructural Nisubstituted spinel ferrites

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Abstract

Ferrites are chemical substances that are obtained as powder or ceramic bodies.Their constituent is iron oxide (Fe_2O_3, FeO), while additional transition metal oxides can alter their characteristics. Nano ferrites $Ni_{(1-x)}Cu_xFe_2O_4$,(x= 0.2,0.4 ,0.5,0.6,0.8) were synthesized by Sol Gel Method withnitrates of Cu, Ni, Fe and citric acid. The X-ray diffraction method (XRD) was used to characterize the structural properties of these materials. Upon Rietveld's refining of these XRD patterns, a well-defined single-phase cubic spinel structure was reconfirmed. With the use of FESEM, the sample's morphology was examined.
Keywords: XRD, Rietveld refinement, FESEM.

A1-0013

Heat transfer characteristics of nanofluid and hybrid nanofluid (Cu-Al_2O_3 /water) flow in porous media in presence of radiation and viscous dissipation.

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Abstract

In the new age of technology for fluids and hybrid nanofluids, the latter has emerged as an attractive interest. The topic is a hot one among researchers because of its properties as well as its potential to produce better results than nanofluids, which can enhance the speed of heat transfer. The goal here is to highlight the significance viscous dissipation and radiation effects on a plate containing a hybrid nanofluid having nanoparticles in aluminum and copper with water as a base fluid. The analysis of hybrid nanofluids is performed in order to incorporate the impact of porous medium, radiation, generating energy flow rate and viscous dissipation on nanoscale materials. The fundamental inner flow region of governing equations is framed as nonlinear coupled partial differential equations via similarity transmutations. The finite element technique (FEM) is employed due to its stability and convergence; outputs are computed using MATLAB code. The impact of physical significance reflective pertinent quantifiers such as, radiation, magnetic field quantifiers, Prandtl, Schmidt, and viscous dissipation quantifiers are illustrated. The velocity and temperature enhances with increasing radiation absorption parameter. It is also observed that an increase of volume fraction of nanoparticles leads to the enhancement of the temperature of the flow and temperature is decreases with the higher values of Pr. The comparison of hybrid nanofluid (Cu-Al_2O_3-water) and copper-water and aluminum-water-based nanoparticles in velocity field, temperature gradient, and species gradient is graphically illustrated. To examine the impacts of the principal flow of heat transfer (Nusselt), skin friction values are tabulated. The rate of heat transfer is higher in hybrid nanofluids compared to mono nanofluids. Additionally, it is observed that HN (Cu-Al_2O_3 water) performs well in heat transmission, making it suitable for cooling applications that boost system efficiency (Heat transfer rate: *normal fluid < nanofluid < hybrid nanofluid).*

A1-0014

Structural and optical studies of ZnO nanoparticles via sol-gel method

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Abstract

The present paper reports on the X-ray diffraction and UV-visible spectroscopy studies of Zinc Oxide (ZnO) nanoparticles (NPs) derived by the sol-gel method. The X-ray diffraction shows the hexagonal structure with maximum diffraction occurring at (101) orientation. The diffused reflectance spectra show a direct band gap transition suggesting an optical band gap of 3.20 eV. The obtained values are suitable for photovoltaic applications.

A1-0016

Effect of Nanoparticle Density on Plasmonic Assembly Size and SERS Enhancements

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Abstract

The surface-enhanced Raman spectroscopy (SERS), a derivative of Raman spectroscopy that achieves signal enhancements, has the potential to detect sample concentrations as low as ppb levels. The SERS can be achieved by keeping the samples on the nanostructured metallic surface or in the locality of metallic nanoparticles (NPs), which serve as SERS substrates. Utilizing the colloidal solution of structured metallic NPs as a SERS substrate offers advantages for analyzing liquid samples, as it generates intraparticle hotspots that significantly improve detection sensitivity. Furthermore, the assembly of metallic NPs in aqueous environments generates multiple interparticle hotspots, contributing to substantial signal enhancement. Over the past few decades, researchers successfully assembled and trapped metallic NPs using various methods. The surface plasmon polariton (SPP) assisted surfactant-free reversible assembly of plasmonic NPs is one of the latest methods, and it stands as a promising approach for conducting SERS measurement on biological samples within an aqueous medium due to its repeatability, reliability, and tunability of the interparticle nanogap. Here, we demonstrated the influence of assembled NP density on SERS intensity. We monitored the change in SERS intensity and assembly size for 60 minutes while assembling NPs in colloidal solutions of varyingNP densities (7.1 to 35.7%). The study revealed that the assembly size remains the same when SERS intensity reaches maxima for every NP density. The average size of the assembled NPs at their maximum SERS intensity was found to be 113±3.5µm. additionally; we demonstrated that the time taken to reach the saturation size of the assembly is inversely proportional to the NP density. This study helps in timing the SERS measurements for optimal signals from the analytes under investigation.

A1- 0017

Impact of Sm insertion on microstructural and magnetic properties of $PrCo_5$ particles with high energy product

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Abstract

$PrCo_5$ particles exhibit promising application potentials in fabricating high-performance permanent magnets and nanocomposite magnets. In view of this, we employ a bottom-up strategy to fabricate highly anisotropic $Pr_{1-x}Sm_xCo_5$ (x= 0 - 0.5) particles. The synthesis process involved mainly two steps, (i) preparation of precursor that contains a mixture of amorphous $Pr(OH)_3$ & $Sm(OH)_3$ and crystalline $Co(OH)_2$ and (ii) Using a calciothermic-reduction, the precursor mixture has converted into $Pr_{1-x}Sm_xCo_5$ particles, which are similar to the traditionally prepared $SmCo_5$ particles. The obtained particles mostly single crystal with an average size from 200nm to 800nm. The single crystal particles assembly show a strong magnetic anisotropy and excellent magnetic properties at room temperature. Consequentially, the best results obtained for x=0.2 are 11.08kOe of H_c, 9.35kG of M_r and 10.82kG of M_s leading to a larger maximum energy product about 18.88MGOe. This enhancement can be instrumental for advanced permanent magnets high storage density applications.

A1- 0018

One-Pot Hydrothermal Synthesis of MoS_2 Phases: Exploring 1T to 2H Transition Under Varying Conditions

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Abstract

The use of transition metal dichalcogenides (TMDs) for energy storage and conversion applications has gained significant popularity. Molybdenum disulfide (MoS2), a prominent TMD, is particularly promising for energy storage devices such as rechargeable batteries and super capacitors due to its unique chemical and structural characteristics. 1T and 2H-MoS_2 were synthesized under varying conditions to optimize energy storage efficiency and examine their surface-enhanced Raman scattering properties. The morphological and chemical features of the MoS2 nanoflowers were examined using various techniques. Phase formation was confirmedby X-ray diffraction (XRD) and Raman spectroscopy. X-ray photoelectron spectroscopy (XPS) was used to analyze the elemental states, while Field Emission Scanning Electron Microscopy (FE-SEM) verified the nanoflower morphology of the synthesized 1T and 2H phases. Additionally, photoluminescence spectroscopy (PL spectroscopy) was employed to confirm the optical and electronic properties of the MoS2 nanoflowers.

A1- 0019

Comparative Analysis Of The Structural Properties Of Cu/Se and Se/Cu Bilayers Irradiated With Low Energy Kr Ion Beam.

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Abstract

The present investigation comprised the sequential e-beam evaporation deposition of Cu (~50nm)/Se (~50nm) and Se (~50nm)/Cu (~50nm) thin films onto silicon substrate. The procedure was performed with a pressure of 2×10^{-5} mbar and at room temperature. Copper selenide, has drawn a lot of interest as a promising thermoelectric material because of its low cost and superior thermoelectric performance. Copper selenide composition usually exists in a wide range of stoichiometric such as CuSe, Cu_2Se, $CuSe_2$, Cu_3Se_2 and Cu_7Se_4. Ion beams of 350 KeV Kr^{+1} were used to irradiate the Cu/Se and Se/Cu bilayers. Recently, thermoelectric thin films have been produced using ion beam processing, which is one of the unique methods for producing thin films. These ion beam-produced thermoelectric films were shown to be nanostructured and to have a higher Seebeck coefficient. The samples were then characterised by XRD, SEM and Rutherford backscattering spectrometry (RBS) to study their structural properties.

Keywords: XRD, RBS (Rutherford Backscattering Spectrometry), SEM.

A1- 0020

Biocompatible Spacer-Gemini Surfactant Mediated Synthesis of PbS Nanoparticles: Aqueous Soft Template Approach with Antioxidant and Antimicrobial Activities

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Abstract

In this study, Gemini surfactants with varying spacer lengths of 12-EDA-12 (g1), 14-EDA-14 (g2) and 16-EDA-16 (g3) were used to synthesize lead sulfide (PbS) nanoparticles to control synthesis parameters, including particle size and shape along with to enhance colloidal dispersibility. The PbS nanoparticles were thoroughly characterized using Energy Dispersive X-ray Analysis (EDAX), Powder X-ray Diffraction (XRD), Raman spectroscopy, Fourier Transform Infrared Spectroscopy (FTIR), Transmission Electron Microscopy (TEM), UV-Vis spectrophotometry, Photoluminescence (PL) and Thermogravimetric Analysis (TGA). The biodegradable gemini surfactant in the forming of PbS nanoparticles played an important role in the morphology of nanoparticles. Structural studies conducted using XRD and Raman spectroscopy revealed that the PbS nanoparticles exhibited a cubic phase. The hydrodynamic size and zeta potential were measured using a Zetasizer providing a thorough understanding of surface features and particle structure. Morphological investigations were carried out using TEM whereas percentage weight loss was determined by TGA. UV–Vis–NIR absorption spectrashowed blue shift compared with the bulk PbS whereas presence of functional groups was confirmed by FTIR. The photoluminescence spectra obtained for PbS nanoparticles shows variation in intensity of sharp emission peak with spacer length of gemini surfactant. The antioxidant properties were evaluated using the 1-diphenyl-2-picrylhydrazyl (DPPH) assay while antibacterial activity was assessed against Gram-positive (*Bacillus subtilis*) and Gram-negative (*Pseudomonas aeruginosa*) using Mueller-Hinton Agar and broth media. The results demonstrate the influence of spacer length on the physicochemical properties and bioactivity of PbS nanoparticles, suggesting potential applications in biomedical and environmental fields.

Keywords: Gemini surfactant, PbS nanoparticles, colloidal stability, antioxidant, antibacterial activity

A1- 0021

Zinc Oxide-Polyaniline Nanocomposite Enriched with Flower Waste for Enhanced Structure and its antibacterial activity against Bacillus subtilis Bacteria

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Abstract

The integration of Zinc Oxide (ZnO) with Polyaniline (PANI) has led to the development of a novel nanocomposite enriched with flower waste, exhibiting enhanced structural and functional properties. This study focuses on synthesising and characterising a ZnO-PANI nanocomposite, incorporating organic constituents derived from flower waste to improve its performance. The incorporation of biowaste not only provides a sustainable approach but also enhances the mechanical and antibacterial properties of the composite. Structural analysis through X-ray diffraction (XRD) and scanning electron microscopy (SEM) confirms the successful integration of ZnO and PANI with the organic material, revealing a uniform distribution and improved crystallinity. The functional properties, particularly the electrical conductivity and thermal stability, were significantly enhanced compared to conventional composites. Furthermore, the antibacterial activity was evaluated against common pathogens, demonstrating a substantial increase in inhibitory effects due to the synergistic action of ZnO and the bioactive compounds in the flower waste. This research underscores the potential of utilizing biowaste in advanced material synthesis, paving the way for eco-friendly and high-performance nanocomposites with broad-spectrum antibacterial applications.

A1- 0022

Nanoscale Zn-Fe2O3: An Excellent Material for Photocatalytic and High Energy Storage Applications

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Abstract

Zinc (Zn) doped nanoscale hematite (α-Fe_2O_3) with varied dopant proportion (pristine, 3%, 5% and 7%) were synthesized via exploding wire technique. X-ray diffraction analysis confirms hematite (α-Fe_2O_3) phase of prepared nanoparticles. The lattice constant and the crystallite magnitude were assessed. X-ray diffraction (XRD) pattern affirmed rhombohedral *R3c* space group of pristine α-Fe_2O_3 nanoparticles with approximate crystallite size of 14nm. The impact of divalent cation (Zn^{+2}) on physical, optical and dielectric performance of α-Fe_2O_3 were investigated. The morphology of nanoscale particles of α-Fe_2O_3 was revealed through scanning electron microscopy. The functional group creation of α-Fe_2O_3 particles and inherent stretching vibration bands of Fe–O were analysed using FTIR results. The Tauc's plot analysis of UV-Vis spectroscopy, exhibited drop in energy band gap up to 5% of Zn content and the contrary trend was observed with further surge in Zn content. The dielectric characteristics of pristine and hematite with Zn dopants were studied at ambient temperature. The dielectric parameters such as dielectric constant (ε′), loss tangent (tan δ), and alternating current (AC) conductivity (σ_{AC}) were investigated. Photocatalytic characteristics of the prepared samples were investigated for unsafe dye. The incidence of UV radiation on hazardous dye showed satisfactorily operative degradation. Hence, α-Fe_2O_3 with impurity of Zn^{2+} can be well thought-out as an effectual material for the unrealized claims in the realm of photocatalysis and increased value of dielectric constant at ambient conditions brands it appropriate for high energy storage equipment.

A1- 0023

Investigate Photoluminescence Properties of Cerium Lanthanide Ions Doped into Cesium Cupric Chloride Nanocrystals

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Abstract

Researchers have focused a lot of attention on CsCuCl3 perovskite because of its great stability and environmental friendliness. However, the process of capturing a charge carrier is primarily controlled by its self-inherent trapping and surface imperfections brought about by strong excitation-phonon coupling. As a result, the photoluminescence's quantum efficiency is significantly decreased, making it impossible to detect the photoluminescent signal and restricting research into its optical characteristics. This work presents the Cerium elements, which were effectively synthesised by the solvent-based thermal synthesis approach, to passivate internal and surface flaws in order to address this issue. This work results in a 52% rise in Cerium doped CsCuCl3 NCs PLQY, which sets a standard for the fabrication of lead-free perovskite optoelectronic devices with good optical characteristics.

A1- 0024

Structural And Optical Analysics of Ag-TiO2/rGO Nanocomposite Via Hydrothermal Route

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Abstract

Noble metal nanomaterials have drawn immense attention due to their unique physio-chemical properties, and they have been widely applied in environment remediation and solar energy conversion. However, photocatalyst nanomaterials have been considered as an appealing option in wastewater treatment to improve purification level, due to their great potential and high efficiency under the irradiation of sunlight for the removal of harmful bacteria and organic pollutants. Silver (Ag) nanoparticle-loaded brookite titanium dioxide ($TiO_{2)}$ nanowires supported on reduced graphene oxide (rGO) were successfully produced by a facile, one-step hydrothermal technique. The properties of fabricated nanowires were analyzed using XRD, FESEM, TEM, HRTEM, XPS, FTIR, Raman, UV–Vis and PL spectroscopy. The present findings recommend that ternary Ag-TiO 2 /rGO nanohybrid provides a promising direction for the development of high quality, effective and reliable photocatalytic and electrode material for organic dyes degradation and hybrid supercapacitors respectively.

A1- 0025

Hot-injection synthesis and characterization of CsPbI3 nanostructures

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Abstract

The cesium lead iodide ($CsPbI_3$) perovskite nanocrystals were synthesized by hot-injection method using cesium carbonate (Cs_2CO_3) and lead iodide (PbI_2) as precursors, 1-octadecane as solvent, and oleic acid and oleylamine ligands as surfactants. XRD pattern indicates the presence of perovskite cubic α-$CsPbI_3$ and orthorhombic black γ-$CsPbI_3$ in the synthesized nanostructures. Literatures show that the cubic α phase and orthorhombic γ phase of CsPbI3 are metastable phases which are stable only at high temperatures. In ambient conditions, these phases spontaneously transform into non-perovskite δ-$CsPbI_3$ phase. The observed stability of the synthesized $CsPbI_3$ in cubic α-$CsPbI_3$ and Black orthorhombic B-γ-$CsPbI_3$ could be due to the nano-scale dimensions of the synthesized nanostructures. FESEM images show the growth of $CsPbI_3$ nanorods. The energy bandgap of the nanostructured $CsPbI_3$ obtained from UV-visible measurement was found to be around 1.73 eV which also indicates the perovskite phase of the synthesized CsPbI3 nanostructures.

A1- 0026

Synthesis and Characterization of Graphene Oxide, Reduced Graphene Oxide, Zinc Oxide, and Reduced Graphene Oxide-Zinc Oxide Nano Composites

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Abstract

Graphene oxide (GO) was prepared by modified Hummer's method and the prepared GO was thermally reduced to reduced GO (rGO) by heating the prepared GO at a low temperature of about 120 ºC for about 72 hours. The XRD pattern confirms the possibility of reduction of GO to rGO by prolonged heat treatment at relatively low temperatures. The FESEM images show two-dimensional sheet like structures of the synthesized GO and rGO. Sol-gel method was used to synthesize ZnO nanostructures which resulted in the growth of nanostructured hexagonal prisms. The ZnO-rGO nanocomposites were prepared by hydrothermal method using a mixture of GO prepared Hummer's method and ZnO nanostructures prepared by sol-gel method dispersed in ethanol solvent by carrying out the growth at 120 ºC for 24 hours. The observation of XRD peaks related to rGO and ZnO in the XRD pattern is one of the indications for the formation of rGO-ZnO nanocomposites. The hydrothermal growth resulted in growth of ZnO nanorods; it appears that the sol-gel synthesized hexagonal prisms act as the seed layers for the growth of nanorods.

A1- 0027

Growth of SWCNTS by PECVD at Low Temperature for the Fabrication of Sensitive Gas Sensor Applications

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Abstract

Here we have grown single wall carbon nanotubes (SWCNTs) on Si substrate by plasma enhanced chemical vapour deposition (PECVD) technique. PECVD method at low temperature. The Fe catalyst was deposited by RF-Sputtering method on Si substrate for the growth of Carbon nano tubes. The Fe deposited Si substrate were subjected into PECVD chamber for the growth of SWCNTs at low temperature (650^0). From the as synthesized SWCNTs highly sensitive chemical sensors were fabricated. The as fabricated sensors were tested for various toxic gases and found highly sensitive towards the trace level detection of toxic gases. Due to high aspect ratio of SWCNTs, they are getting much importance in gas sensing applications. For surface and structural characterization, Field emission scanning electron (FESEM) and Raman Spectroscopy were used. High quality SWCNTs were observed in FESEM and the diameter distribution was observed about 1-2 nm by Raman Spectroscopy. The as fabricated sensors were tested for various sensing characteristics like fast response /recovery, high sensitivity, repeatability, and long-term stability.

Keywords: SWCNTs, VA-SWCNTs; RO-SWCNTs; Gas sensing; Sensor Characteristics; PECVD etc.

A1- 0028

A new Synthesis approach of Graphene-like Nanosheets via Single-Step Thermal Exfoliation

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Abstract

Graphene's remarkable electrical, mechanical, sensing, and thermal properties have captured the attention of researchers worldwide and revolutionized the field of material science. However, traditional synthesis methods, such as Hummer's method, require the use of harsh chemicals, lengthy procedures, and the release of dangerous gases. These processes are expensive, complicated, and insensitive to the environment. We offer a creative, affordable, and environmentally responsible answer to these issues. Our group has developed a straightforwardphysical method that produces graphene-like nanosheets by thermally exfoliating bulk graphite in a single step. Using traditional methods is less complicated and costly, and dangerous chemicals are not needed. In order to evaluate the characteristics of the synthesized graphene- like nanosheets, we carried out comprehensive physiochemical characterizations utilizing state- of-the-art techniques such as Raman spectroscopy, X-ray diffraction (XRD), Brunauer-Emmett- Teller (BET) surface area analysis, scanning electron microscopy (SEM), and transmission electron microscopy (TEM). These studies showed that the nanosheets feature numerous dots, a highly crystalline structure, and an impressive surface area. Our initial results indicate that the one-step thermal exfoliation approach is highly scalable and ecologically benign, making it perfect for producing graphene-like nanosheets on a wide scale. The remarkable structural and electrical characteristics of the synthesized material present promising opportunities for sensors, energy storage devices, and flexible electronics applications. Thanks to this straightforward and environmentally benign approach, more effective and eco-friendly ways of manufacturing graphene will now be feasible, marking a major breakthrough in the field.

A1- 0029

Effect of silver incorporation on structural and optical properties of TiO2 thin films prepared via non-aqueous sol-gel route

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Abstract

Pure, 4 at%, 8 at%, 12 at%, and 16 at% Ag-doped TiO_2 thin films were fabricated by spin coating technique using a non-aqueous sol-gel method. The effect of Ag doping on the structural and optical properties of TiO_2 thin film has been investigated using X-ray diffraction (XRD), Raman spectroscopy, scanning electron microscopy (SEM), UV-visible (UV-Vis) spectroscopy, X-ray photoelectron spectroscopy (XPS) and photoluminescence (PL) spectroscopy. Using XRD and Raman spectroscopy, it was found that PT, 4AT, 8AT, and 12AT thin films showed pure anatase phase while 16AT film showed mixed anatase and rutile phase. XRD analysis revealed that an increase in Ag content reduces the transition temperature from the anatase-to-rutile phase. UV-Vis spectroscopy revealed that the band gap reduced from 3.2 eV in the PT to 2.6 eV in the 12AT sample. X-ray photoelectron spectroscopy (XPS) confirmed the presence of both Ag^0 and Ag^+ states in the 12AT sample, suggesting partial doping of Ag^+ and the presence of metallic Ag as well on the surface of TiO_2 thin films. XPS and PL spectroscopy results confirmed the formation of oxygen vacancies and reduction in recombination centers, being the highest in the 12AT sample. The photocatalytic activity evaluated using degradation of RhB dye under visible light irradiation showed that, with an increase in Ag doping, photocatalytic activity increases. The highest photocatalytic activity of the 12AT sample could be attributed to its pure anatase phase, presence of oxygen vacancies, and reduction in e^--h^+ recombination rates.

A1- 0030

Investigation on the Structure and Enhancement in the Photoluminescence Properties of Li-co-doped MgAl2O4:Tb3+/PVP Capped Nanophosphors for Solid State Lighting Applications

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Abstract

Lanthanide activated fluorescent nanophosphors are in great demand due to their enormous application in optical devices, field emission displays, light emitting diodes, solar cells etc. Rare earth based nanophosphors have numerous advantageous properties such as long lifetime, high energy efficiency, better quantum yield, great reliability and environmentally friendly characteristics. In the present study, green light emitting Mg1-xAl2O4: Tb_x^{3+}, (x = 0.02, 0.04, 0.06, 0.08 and 0.1) and Li-co-doped $MgAl_2O_4:Tb^{3+}$ nanophosphors have been synthesized by *Polyvinylpyrrolidone* (PVP) polymer capped sol-gel combustion method. PVP primarily acts as capping and stabilizing agent, controlling the growth and preventing particle aggregation during synthesis. Structure, morphology and luminescence dynamics of the synthesized phosphors depends on the Tb^{3+} doping concentration. The emission spectra exhibit several peaks corresponding to $^5D3 \rightarrow {}^7FJ$ (J=4 and 5) and $^5D4 \rightarrow {}^7FJ$ transitions (J=3, 4, 5 and 6). Among them, the most prominent transition is the $^5D4 \rightarrow {}^7F5$ transition (543 nm), which is responsible for the green colour observed in the focused nanophosphor samples. In-corporation of Li^+ ions resulted in the enhancement of photoluminescence properties and better emission features of the prepared nanophosphors. Photoluminescence emission intensity of Mg1-x-yTbx LiyAl2O4 (x = 0.04, y=0.05) is found to be enhanced to about 1.9 times that of the optimal Mg0.96Tb0.04Al2O4 nanophosphor with a slight increase in the asymmetric ratio value. The decay profiles of all the prepared nanophosphors exhibit double exponential behaviour withincrease in the lifetime values with Tb^{3+} ion concentration. Further, the Dexter's theory provides valuable insights into the concentration quenching mechanism observed in the prepared nanophosphors. The confirmation of emission in the green region, as indicated by CIE colour co-ordinates, validates that the synthesized Mg1-xTbxAl2O4 (x = 0.02, 0.04, 0.06, 0.08 and 0.10) and Mg1-x-yTbx LiyAl2O4 (x = 0.04, y=0.05) nanophosphors as suitable candidates for green component integration in phosphor based high-quality lighting applications.

A1- 0031

Investigation of Structural Parameters and Enhanced Photocatalytic Activity of ZnO-GO Nanocomposites

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Abstract

The development of ZnO-GO (Zinc Oxide-Graphene Oxide) nanocomposites has sparked considerable interest due to their potential applications in environmental remediation, particularly in photocatalysis. This research focuses on a comprehensive investigation of the structural parameters and enhanced photocatalytic activity of ZnO-GO nanocomposites. By employing a simple synthesis method, we aim to optimize ZnO-GO nanocomposites for photocatalysis. Advanced characterization techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM), were utilized to analyze the crystallinity, particle size, morphology, within the ZnO-GO nanocomposites. These structural investigations revealed that the incorporation of GO significantly influences the crystallinity and thereby affecting its functional properties. The photocatalytic performance of the ZnO-GO nanocomposites was evaluated through the degradation of organic pollutants (Methylene Blue) under UV and visible light irradiation. The results demonstrated a substantial enhancement in photocatalytic activity compared to pure ZnO, attributed to the synergistic effects between ZnO and GO. The GO component effectively facilitated the separation of photo generated electron-hole pairs and provided additional active sites for photocatalytic reactions, leading to improved light absorption and reduced electron-hole recombination. This study provides valuable insights into the structural and functional interplay between ZnO and GO. The findings underscore the potential of ZnO-GO nanocomposites for practical applications in environmental remediation, offering a pathway for the development of advanced photocatalytic materials with tailored properties.

Keywords: Zinc Oxide, Graphene Oxide, nanocomposites, Photocatalysis

A1- 0032

Synthesis and Electrochemical Properties of Eu-Doped CuO Nanoparticles for High-Performance Supercapacitors

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Abstract

Supercapacitors are promising energy storage devices due to their high power, fast charge-discharge rates, and long lifespan. Copper oxide (CuO) is a cost-effective electrode material with good redox properties. In this work, the electrochemical properties of europium (Eu) doped CuO nanoparticles were studied. The undoped and Eu-doped CuO nanoparticles were synthesized using a facile co-precipitation method. The prepared nanomaterials were investigated using X-ray diffraction (XRD), scanning electron microscopy (SEM), electron dispersive spectroscopy (EDS), and electrochemical measurements. XRD and SEM analyses show that the incorporation of Eu into CuO significantly affects the crystal structure and morphology of the CuO nanoparticles. Further, electrochemical measurements show a remarkable improvement in electrochemical properties after Eu-doping, showing enhanced specific capacitance and cyclic stability. The study highlights the potential of Eu-doped CuO nanoparticles as electrode materials for high-performance supercapacitors.

A1- 0033

Probing the structure and photoluminescence properties of CaZrO3:Eu3+ nanophosphors synthesized by PVA assisted sol-gel method

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Abstract

Rare earth doped inorganic luminescent materials have great potential for use in photonic and optoelectronic applications such as solid-state lasers, high-resolution displays, pcLEDs, solar energy converters and medical imaging. The effectiveness of rare earth activators depends significantly on the host material, which facilitates their excitation and enhances emission. Calcium zirconate ($CaZrO_3$), a perovskite with disordered orthorhombic structure, is an excellent host due to its high stability, wide band gap, superior dielectric, diverse physical-chemical and photoluminescence properties. In the present study, highly luminescent red emitting $Ca_{1-x}Eu_xZrO_3$ (x = 0.02, 0.04, 0.06, 0.08 and 0.10) nanophosphors were synthesized by polyvinyl alcohol (PVA) assisted controlled sol-gel combustion method. X-ray diffraction and Rietveld refinement confirmed the successful incorporation of Eu^{3+} in $CaZrO_3$ lattice. TEM micrographs indicated the formation of nearly spherical shaped $CaZrO_3:Eu^{3+}$ nanophosphors. Fourier transform infrared and microRaman spectroscopic measurements showed the characteristic vibrational modes of $CaZrO_3$. Optical band gap evaluated by Kubelka-Munk method from the diffuse reflectance spectra gets decreased with increase in Eu^{3+} concentration. Photoluminescence studies exhibited strong absorption at 395 nm and intense red emission at 615 nm corresponding to the hypersensitive forced $^5D_0 \rightarrow {}^7F_2$ electric dipole transition of Eu^{3+} ions. Emission intensity decreased beyond 8 mol.% Eu^{3+} concentration due to concentration-dependent quenching and increased non-radiative transitions. Luminescence decay curves followed single exponential behaviour and the observed lifetime was found to decrease as the Eu^{3+} concentration increases. CIE chromaticity coordinates of all the nanophosphors lie in the red region with a correlated colour temperature of 1716 - 2307 K. The culminated results suggest the potential use of $Ca_{1-x}Eu_xZrO_3$ nanophosphors as efficient warm red-emitting material for various optoelectronic and photonic applications.

A1- 0034

Comparative Study of Radiation Shielding Parameters for NiCuFe2O4 and NiMgFe2O4 Nanoparticles.

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Abstract

This work employed the Sol-gel auto-combustion process to produce ferrite samples of NiCuFe2O4 and NiMgFe2O4. Various analytical methods were employed to examine the synthetic materials' structural, optical, and functional groups, including XRD, UV-Vis, and FTIR. Furthermore, we examined the gamma-ray shielding characteristics for the produced materials using a NaI (Tl) scintillation detector and a variety of gamma-ray sources. The theoretical values and the experimental results exhibited a strong connection. This software program evaluated the synthesized ferrite nanoparticles' capability to shield against gamma radiation. By adjusting the radiation dose's strength, ferrites have been exposed to gamma radiation from an array of sources. An investigation of the mass and linear attenuation coefficients, mean free path, half value layer, tenth value layer, effective atomic number, and effective electron density for synthesized spinel ferrites at 122–1330 keV is conducted using Phy-X/PSD software. The gamma-ray energy absorption build-up factor (EABF) for selected ferrites is investigated at incident photon energy levels ranging from 0.015 to 15 MeV using the geometric progression (G-P) fitting technique. It is widely recognized that the recommended nanoparticles can aid in improving shielding against γ-radiation.

A1- 0035

An Sm^{3+} activated $K_2MgP_2O_7$ nanophosphor: Synthesis, Structural, Optical, and Photoluminescence Studies

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Abstract

The incandescent and fluorescent lamps are replaced by new generation solid-state lighting as these smart light sources can alter according to the specific requirements and have potential in the field of lighting, automobiles, transportation, agriculture and medicine [1]. Phosphates are widely used because of its exceptional simplicity, low manufacturing cost, low viscosity, high UV absorption, thermal constancy, isotropic refractive index, and simple synthesis [2]. In this study, the solution combustion approach is opted to synthesize the undoped and Sm^{3+} doped $K_2MgP_2O_7$ nanophosphor. The synthesized material is subjected to structural, optical, and photoluminescence spectroscopy studies. For the structural analysis, XRD diffracted peaks were compared with the JCPDS card no. (52-1084) and observed that the diffracted peaks are in complete agreement. Using Debye- Scherrer formula the average crystallite size is estimated to be 45 *nm* and 41 *nm* for the undoped and doped material. The optical bandgap is calculated from analyzing DRS spectra by Kubelka Munk function and values comes out to be 3.95 eV and 3.87 eV for undoped and Sm^{3+} doped $K_2MgP_2O_7$ material In the PL emission spectra, the four peaks positioned at 564, 601, 646, and 704 *nm* are recorded at λ_{exc}= 402 *nm*. The photometric analysis reveals that the CIE coordinates are (x = 0.59, y = 0.40) which indicates the emission in the amber region of the color spectrum. The CCT has a value of 1553.44 *K* and the color purity of the synthesized phosphor is 91%. These results indicate the possible application of the synthesized phosphor in solid-state lighting as amber LEDs.

Keywords: XRD, PL, UV-Vis.

A1- 0036

Optimization of dielectric response of Al_2O_3/PVDF nanocomposites

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Abstract

In this contribution we are presenting dielectric response of Al2O3/PVDF nanocomposites synthesized by solution casting method. By dissolving PVDF in a suitable solvent and incorporating Al_2O_3 nanoparticles, a uniform dispersion is achieved, leading to enhanced dielectric and mechanical properties. The solution casting process facilitates the formation of well-dispersed Al_2O_3 nanoparticles within the PVDF matrix, which significantly improves the composite's dielectric constant and energy storage density. Dielectric response indicating that incorporation of Al_2O_3 nanoparticles leads to a notable increase in capacitance and energy density, making these nanocomposites ideal for high-performance supercapacitors and other energy storage applications. The abstract also discusses the scalability of the solution casting method and its potential impact on the commercialization of Al_2O_3/PVDF nanocomposites in energy storage technologies.

A1- 0036

L-Tyrosine Capping Agent-Induced Synthesis of Zinc Oxide Nanostructures and Study of Optical Properties

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Abstract

Zinc Oxide nanostructures (ZnO-NSs) of different morphologies are synthesized with the amino acid L-Tyrosine as capping agent in aqueous medium at different temperatures. In growth mechanism, L-Tyrosine and temperature play important roles in the formation of ZnO NSs. The X-Ray diffraction (XRD) and transmission electron microscopy (TEM) investigations show that ZnO NSs possess good crystalline structures with growth directions along the polar planes i.e. (0001) and (000$\bar{1}$). Ultraviolet-visible spectroscopy (UV-vis) results showed a blue shift in absorption peaks. The method provides a simple route to control the length and shape of ZnO nanorods for potential applications in various fields.

A1- 0037

Synthesis and Characterization of Nanocrystalline MgFe2O4 for Multifaceted Applications

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Abstract

Nanocrystalline spinel ferrites have garnered considerable interest from researchers due to their unique structural, magnetic, and electrical properties. The enhanced characteristics of nanomaterials are attributed to their high surface-to-volume ratio. Alterations within the spinel lattice and variations in nanoparticle size significantly influence key parameters such as Curie temperature, electrical resistivity, magnetic moment, and lattice constants. This study focuses on the fabrication of nanocrystalline $MgFe_2O_4$ for various applications, including Electromagnetic Interference (EMI) shielding, sensors, data storage, solar cells, and magnetic drug delivery. The sol-gel method was employed, using varying amounts of citric acid to synthesize $MgFe_2O_4$ ferrite samples. X-ray diffraction (XRD) analysis revealed a single cubic phase structure, with broad peaksindicating nano-sized particles. By applying the Debye-Scherrer formula, it was observed that anincrease in citric acid content led to a decrease in full width at half maximum (FWHM) broadening, as reflected in the XRD patterns. Field Emission Scanning Electron Microscopy (FE- SEM) was used to study surface morphology, showing well-formed spherical particles in all samples. Furthermore, Energy Dispersive Spectroscopy (EDS) confirmed the elemental composition, verifying successful doping in the polycrystalline samples. Fourier Transform Infrared Spectroscopy (FTIR) further confirmed the presence of various chemical bonds.

A1- 0038

Crack Angle Distribution in Granular Materials

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Abstract

Desiccation of granular materials is usually accompanied by isotropic contraction and shrinkage of the medium, often resulting in polygonal shapes. The size and shape of the cracks, and thus the pattern left behind, is a function of (i) the type of material undergoing desiccation, (ii) water content and evaporation dynamics of the system (iii) conditions of the environment (iv) inhomogeneities in the system and (v) boundary conditions. When the water content, boundary conditions, and environment are held constant, and the system is assumed to be homogeneous, the desiccation crack patterns are a function of the nature of the system. In this study, we report the nature of desiccation cracks taking the example of soil as granular material. The images of the desiccation cracks are analyzed through a study of their crack angles and the distributions that they follow. Three different types of soils namely, clay, sandy-clay-loam, and silt, from the Brahmaputra basin, are studied for the distribution of crack angles in the desiccation cracks. The results show the predominance of closed polygons in clay, reflective of the fine particle size of clays in comparison to others, leading to low evaporation rates. Also, the desiccation cracks commonly form 3, 4, 5, 6, and 7-sided polygons, with 4-sided polygons being the most abundant, as is often observed. Moreover, the fracture morphology results in polygonal patterns, with the crack tips terminating when they intersect with other cracks or the sample edge. A distinct bimodal distribution of crack angles is seen in the case of sandy-clay-loam, indicative of the mixed nature of the soil.

A1- 0039

Plasmon-Induced Giant Photoluminescence Enhancement and Tunable Emission Wavelength in MXene-Metal Nanoparticle Heterostructures

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Abstract

This study investigates the enhanced photoluminescence (PL) and redshift in emission wavelength resulting from the nanocomposite of MXene nanosheets with metal nanoparticles. MXenes, a class of 2D transition metal carbides, are known for their excellent electrical conductivity and optical properties. By integrating Nb2C MXene nanosheets with metal nanoparticles, we observed a significant enhancement in photoluminescence, attributed to the localized surface plasmon resonance (LSPR) effect of the metal nanoparticles. The hybrid structures were synthesized through a sonication-assisted process, ensuring uniform dispersion of the nanoparticles on the MXene surface. Scanning electron microscopy (SEM) confirmed the successful decoration of MXene nanosheets with metal nanoparticles, revealing a uniform distribution across the surface. Photoluminescence (PL) spectroscopy showed a remarkable increase in emission intensity compared to pristine MXene, with a distinct redshift in the emission wavelength. This shift is likely due to the interaction between the excitonic states of MXene and the LSPR of the silver nanoparticles, resulting in energy transfer and recombination at lower energy levels. The synergistic effect of MXene's 2D structure and the plasmonic properties of metal nanoparticles pave the way for advanced optoelectronic applications, particularly in sensing, imaging, and light-emitting devices. The results demonstrate that MXene/metal nanoparticle heterostructure holds promise for engineering photonic devices with tunable optical properties.

A1- 0040

Exploring Structural, Optical, Dielectric and Ferroelectric Properties of Cobalt Doped Barium Calcium Titanate (BCT)

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Abstract

Ceramic samples of cobalt doped barium calcium titanate (BCT) ($Ba_{0.80}Ca_{0.20}Ti_{1-x}Co_xO_3$with x =0.000, 0.005, 0.010, 0.015, and 0.020) were synthesized using the standard solid-state reaction method. These samples were then examined for structural, microstructural, dielectric, optical, and ferroelectric characteristics analyses. Through rietveld refinement of X-ray diffraction patterns, the tetragonal structure with the space group P4mm has been verified for each of the produced samples. Micrographs obtained through Field Emission Scanning Electron Microscopy (FESEM) showed that the typical particle size is in the micrometer range of 0.3µm -0.8µm. Optical analysis shows that the energy bandgap gradually decreased as the doping concentration increased from 3.31 eV to 2.71eV. At room temperature, dielectric properties with varying frequencies showed a decreasing trend. P-E loop measurement shows the increase in maximum polarization and remnant polarization of the ceramic with the increased in applied electric field.

Keywords: BCT, Rietveld refinement, Dielectric, Ferroelectric properties.

A1- 0041

Mechano-Chemical Synthesis of Metal Oxide Nanoparticles via Solvent-Free Solid State Reaction

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Abstract

Mechano-chemical synthesis offers a solvent-free, solid-state approach for the production of metal oxide nanoparticles. This method involves the use of mechanical grinding via ball milling, bead mill, attrition milling or manual grinding to induce chemical reactions, avoiding the need for liquid solvents. In this study, mechano-chemical technique was employed to synthesize Fe2O3, Al2O3, Co3O4, and ZnO nanoparticles. The process involved the solid-state reaction of hydrated metal salts with ammonium or sodium bicarbonate, followed by grinding in a mortar and pestle to form hydroxides, which were then calcined at high temperatures to produce the desired metal oxides. Comprehensive characterization was conducted using X-ray diffraction (XRD), thermogravimetric analysis (TGA), differential thermal analysis (DTA), differential scanning calorimetry (DSC), and scanning electron microscopy (SEM). These techniques allowed us to assess the crystal structure, phase purity, thermal stability, and morphology of the synthesized nanoparticles. The results highlight the effectiveness and versatility of the mechano-chemical synthesis method, offering a promising alternative for the industrial-scale production of metal oxide nanoparticles.

Keywords: Mechano-chemical synthesis, Metal oxide nanoparticles, Solid-state reaction, Catalysts

A1- 0042

Investigate the Effect of Ni and Cu Doping on ZnO nanoparticles Synthesized by Solution Combustion Method Towards Antimicrobial Activity and Photocatalytic Degradation of Methylene Blue Dye

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Abstract

The green solvent solution combustion method was effectively used to produce $Zn_{1-x}Ni_xO$ and $Zn_{1-x}Cu_XO$. The structural, morphological, and optical properties of the produced materials were investigated using XRD (X-ray diffraction), SEM (scanning electron microscopy), EDX (energy-dispersive X-ray), Raman Spectroscopy, and UV-Vis diffuse reflectance spectroscopy. The photocatalytic activity of the synthetic materials was investigated in relation to the degradation of methylene blue dye under UV light irradiation. $Zn_{1-x}Cu_XO$ was found to be the most efficient photocatalyst among the compounds under investigation, degrading 83% of the dye after two hours of exposure to light. Investigations were conducted into the impact of operational parameters on the degradation percentage, including pH, starting dye concentration, and catalyst dosage. To ensure the stability of the samples for long-term application, a reusability test of the photocatalyst was also conducted. Further, the antibacterial activity against both Gram-negative and Gram-positive bacteria was evaluated through analysis of zone of inhibition and microscopy images. Among the prepared nanostructures, the $Zn_{1-x}Cu_xO$ sample showed excellent antibacterial activity against gram positive bacteria. The potential photocatalytic and antibacterial activity of synthesized nanomaterials makes them useful for environmental remediation.

Keywords: Solution combustion synthesis, Green Solvent, Photocatalytic Activity, Antimicrobial Activity

A1- 0043

Enhancing the properties of Sb_2Se_3 Thin Films for Photoelectrochemical Water Splitting: Effects of Annealing on Structural and Optical Properties

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Abstract

Antimony selenide (Sb_2Se_3) is a promising material for photoelectrochemical (PEC) water splitting due to its favorable electronic properties and tunable band gap. This study explores the effects of annealing on Sb_2Se_3 thin films deposited via thermal evaporation. The films were annealed at temperatures ranging from 150°C to 350°C to enhance their crystallinity, morphology, and band gap. Characterization through X-ray diffraction (XRD), scanning electron microscopy (SEM), and ultraviolet-visible (UV-Vis) spectroscopy revealed that higher annealing temperatures improved film crystallinity, resulting in larger, more uniform grains and smoother surfaces. The band gap varied from approximately 1.1 eV to 1.5 eV, depending on the annealing temperature. Films annealed at 300°C exhibited the best combination of improved structural quality and optimal band gap for PEC applications. These films achieved superior photocurrent density and onset potential in PEC water splitting tests, indicating enhanced performance for hydrogen production. The study demonstrates that precise control of annealing conditions can significantly enhance the properties of Sb_2Se_3 films, making them highly suitable for efficient and sustainable PEC water splitting applications.

A1- 0044

Electrochemical study on role of PEDOT-PSS in ZnO NP's based Super Capacitor

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Abstract

In this study, we investigate the super capacitor behavior of zinc metal oxide (ZnO) combined with PEDOT-PSS polymer. The synthesis of the ZnO-PEDOT-PSS composite was carried out through a facile and scalable chemical method, ensuring uniform dispersion of ZnO nanoparticles within the PEDOT-PSS matrix the electrochemical performance of the ZnO-PEDOT-PSS composite was evaluated through Cyclic voltammetry (CV), Galvanostatic charge-discharge (GCD), and Electrochemical impedance spectroscopy (EIS). The electrode exhibited remarkable specific capacitance, which can be attributed to the synergistic effect between ZnO and PEDOT-PSS. ZnO nanoparticles provide a high surface area and facilitate fast electron transport, while PEDOT contributes to the overall conductivity and mechanical stability of the electrode. Moreover, the ZnO-PEDOT composite showed a significant electrochemical performance, surpassing those of individual ZnO or PEDOT electrodes.

A1- 0045

Electrochemical Study on role of PEDOT: PSS in Vanadium based Ternary Metal Oxide nanoparticle Supercapacitor

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Abstract

In this study, we examine the vanadium-based ternary metal oxide (ZnO: MnO:VO) synthesis by hydrothermal technique in combination with PEDOT-PSS polymer for supercapacitors. The electrochemical performance of the TMO-PEDOT-PSS composite was assessed using cyclic voltammetry (CV), Galvano static charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS). The synergistic action of TMOs and PEDOT-PSS resulted in an electrode with a remarkable specific capacitance. TMO nanoparticles have a large surface area and allow for rapid electron transport, PEDOT improves the electrode's total conductivity and mechanical stability. Furthermore, the TMO-PEDOT composite had much greater electrical –chemical performance than individual TMO or PEDOT electrodes. In conclusion, the TMO-PEDOT composite shows significant promise as an improved material for electrodes in high-performance super capacitors

A1- 0046

Synthesis and photoluminescence studies of highly efficient vanadium oxidenanorods for photodetector application

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Abstract

Highly cost-effective synthesis approach has been adopted to prepare stable V_2O_5 nanorods for energy storage device application. The as-synthesized nanorods are thoroughly characterized using advanced techniques, including scanning electron microscopy (SEM), X-ray diffraction (XRD), UV visible and photoluminescence (PL). The mentioned techniques were performed to provide the valuable insight into the morphological, structural, optical and photoluminescence properties of as-synthesized V_2O_5 nanorods. X-ray diffraction exhibit the structural properties with the highest bragg's angle observed at 8.66 degree. Surface morphology of the as-prepared and calcinated nanorod's samples was studied by using the scanning electron microscope (SEM). The observed bandgap of NRs was calculated using tauc plot and achived at 2.61 eV. The photoluminescence spectroscopy demonstrates the luminescence behaviour of as-synthesized nanorods. Aforementioned synthesis and results achieved through characterizations exhibits its potential suitability for photodetector applications.

Keywords: V_2O_5, Hydrothermal, Nanorods (NRs), Photodetector

A1 -0047

A Novel Method For Spatially-Selective ZnO Thin Film Growth By The Sol-Gel Technique

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Abstract

Sol-gel deposition of ZnO using the dip-coating method typically generates uniform large area thin films on various substrates, and individual devices are created by a subsequent etching step. In this paper a method for the spontaneous formation of islands of ZnO aligned to existing electrode structures has been presented. Ring-type platinum electrodes with dimensions ranging from 200mm to 800mm were initially fabricated on to sapphire substrates using standard photolithographic process steps. Subsequently a ZnO thin film was grown on to the patterned substrate by sol-gel using the dip-coating technique. Finally, ZnO nanowires were deposited by the vapor-liquid-solid process. The films were evaluated by optical microscopy, SEM and EDS imaging methods. The results indicate that difference in wettability of the platinum and sapphire areas of the wafer by the precursor solution during the dip-coat process leads to the spontaneous formation of spatially-selective structures of ZnO. Specifically, along with a uniform thin coating of ZnO, thicker islands were formed inside the platinum electrode ring, which avoid proximity to the electrode edge. The morphology of these islands shows a honeycomb-like pattern with extended ridges. The density and nature of the VLS-grown ZnO nanowires depend on the underlying thin film, and are observed on the top of the ridge-like structures, thereby enhancing the surface area. This approach is well suited for formation of ZnO-based sensor devices. Spatial selectivity of the deposition allows the development of semiconductor devices while eliminating the need of any chemical etching process step.

A1- 0048

Facile synthesis and magnetic properties of chromium oxide nanoparticles

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Abstract

The synthesis of Cr_2O_3 nanocrystal has been done *by chemical precipitation method using ammonia as a precipitating agent.* The rhombohedral crystal structure and single crystalline nature of Cr_2O_3 powder were verified by X-ray diffraction (XRD) analysis. The Debye-Scherrer formula was utilized to ascertain the average size of crystallites. The structure and morphology of Cr_2O_3 nanoparticles were examined using scanning electron microscopy (SEM). The various functional groups in Cr_2O_3 nanoparticles were identified by the Fourier transform infrared spectroscopy (FTIR) findings. Using a vibrating sample magnetometer (VSM), the antiferromagnetic (AFM) behavior of Cr_2O_3 nanoparticles was investigated. These finding suggests that the synthesized nanocrystal may be used in quantum computing, data storage, and magnetic sensors.

Keyword: Cromium oxide nanoparticles (Cr_2O_3), X-ray diffraction (XRD), SEM, VSM.

A1- 0049

Dehydration Kinetics of Maltose Monohydrate by Iso-conversional methods

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Abstract

The dehydration kinetics of maltose monohydrate is studied by thermal analysis tool, differential scanning calorimetry (DSC) at different heating rates (1, 2, 4, and 8 K/min) under non-isothermal mode. Four iso-conversional approaches (Starink, Tang, Ozawa-Flynn-Wall and Kissinger-Akahira-Sunose) were utilized to determine different kinetic parameters: Fractional crystallization (α), crystallization temperature(T_α), activation energy of dehydration(E_α),Avrami exponent(n_α),pre-exponential factor(A_α),as well as changes of entropy($\Delta S^{\#}$), enthalpy ($\Delta H^{\#}$),and Gibbs free energy($\Delta G^{\#}$) in non-isothermal condition. The activation energy of dehydration (E_α) for the four methods calculated is in the range of 375 – 335 kJ/mol and is in agreement with the earlier reported values in the literature. Lastly, comparison of the accuracy and applicability of different iso-conversional methods are discussed.

A1- 0050

P/N-type AgO-Chitosan biosensor for sensing hydrogen to detect gastro-intestinal diseases.

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Abstract

Our report study describes study of AgO:Chitosan [A(1:2), B(1:1), C(1:0.5), D(1:0.25), E(1:0.125), F(1:0.0625)] based hydrogen sensor for detecting gastrointestinal diseases at RT. AgO:Chitosan ratios were synthesized by novel co-precipitation cum probe sonication technique and characterized by XRD,UV-VIS,FTIR,RMAN,FESEM,TEM. Among the six synthesized ratios the composite which can detect lowest (0.2-10) ppm of hydrogen will be further analysed by studying its sensitivity, response, recovery, reproducibility, stability, and selectivity. Using Hall effect the composites P/N type nature will be determined. The reaction mechanism for sensor performance and its P/N type nature elaborately discussed. The above studies will suggest reveal a new material AgO:Chitosan for hydrogen sensors that can be used for the breath analysis to detect GIDs.

A1- 0051

Structural, Optical and Magnetic Properties Analysis of Fe Doped Gd_2O_3 Nanoparticles Route: Hydrothermal

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Abstract

In this study, the authors utilized a cost-effective hydrothermal approach to produce nanoparticles of Gd_2O_3 and Fe-doped Gd_2O_3 with Fe concentrations ranging from 1% to 5%. A range of complementary analytical techniques, including TEM, SEM, XPS, XRD, Raman, FTIR, VSM, UV-Vis, PL, photocatalytic, and electrochemical analyses, were employed to characterize and evaluate the nanoparticles. XRD analysis revealed that all samples exhibited a pure cubic phase with crystallite sizes typically between 25 and 35 nm. SEM and TEM images showed that the nanoparticles had a spherical shape with average diameters between 8 and 12 nm. A redshift in the optical absorption edge with increasing Fe_3+ ion concentration indicated a reduction in the energy band gap of the nanoparticles from 3.34 eV to 3.04 eV. VSM measurements revealed that all samples exhibited paramagnetism at both 5 K and room temperature, within a magnetic field range of -60 to +60 kOe. The photoluminescence (PL) emission properties of pure and Fe-doped Gd_2O_3 were examined in the 301 to 651 nm range. Excitation at 276 nm resulted in a PL emission band in the ultraviolet region (317 to 371 nm) as well as emissions in the blue, green, and red regions. Compared to pure Gd_2O_3 nanoparticles, the Fe(5%)-doped Gd_2O_3 nanoparticles demonstrated superior photocatalytic activity, which could be attributed to enhanced light absorption, reduced electron-hole pair recombination, and a narrower optical band gap.

A1- 0052

Electronic Properties Of Two-Dimensional C_6B_4 And Its Application In Hydrogen Storage Using Density Functional Theory

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Abstract

Storing hydrogen and its release at ambient conditions has been a major challenge in developing the hydrogen energy technology. Here, we are presenting first-principles calculations based on density functional theory for monolayer of C_6B_4 using Perdew-Burke- Ernzerhof (PBE) form of generalized approximation (GGA) in order to explore its potential in application of hydrogen storage. Monolayer of C_6B_4 stabilizes in a planar structure in an orthorhombic unit cell having lattice constants a=5.35 Å, b =6.28 Å and c=20 Å, comprising of 6 carbon and 4 boron atoms. Electronic structure calculations confirm that it exhibits metallic character and the valence and conduction band edges are formed by C-2p and B-2p orbitals. There are total six sites suitable for adsorption of H_2 molecule, out of which the largest hollow site has adsorption energy of -0.91 eV which is energetically the most favorable whereas the least favorable site is when H_2 molecule is adsorbed on carbon atom with adsorption energy of - 0.2 eV. The average desorption temperature corresponding to most and the least favorable site is found to be 672 K and 148 K respectively. Due to availability of a variety of sites, the material can adsorb large number of H_2 molecules resulting in higher storage capacity. Our results suggest that C_6B_4 monolayer is viable for its application in hydrogen storage.

A1- 0053

1T-TaS_2 2D-monolayer: An *ab-initio* study of Li adsorption.

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Abstract

Two-dimensional (2D) materials have garnered significant attention in materials research due to their superior physical and chemical properties. This study employs density functional theory (DFT) with the Vienna *ab-initio* Simulation Package (VASP) for the study of 2D monolayer of 1T-TaS_2. 1T-TaS_2 in its bulk form is a layered material having trigonal prismatic structure (P3m space group) in which the monolayers are held together by van der Waals forces. We started with geometric structure optimization of the bulk and the monolayer followed by evaluation of electronic band structures and density of states (DOS) using the generalized gradient approximation with the Perdew–Burke–Ernzerhof (GGA-PBE) functional incorporating spin-orbit coupling and van der Waals interactions. Our results reveal that the lattice parameters and electronic properties of the 2D monolayer deviate very slightly from the bulk phase, inheriting the metallic character contributed by Ta-5d and S-3p orbitals. Ionic- relaxation calculations reveal that Li-ion stabilizes at three distinct sites with energies ranging from 0.005 eV to -1.06 eV and adsorption heights (measured from the top layer of sulphur atoms) in therange 1.3Å to 1.8Å. Bader charge analysis implies a charge transfer of $0.86e^-$ from the Li-ion to the monolayer. Additionally, the climbing image-nudged elastic band (CI-NEB) method is used to investigate the transport properties revealing a low diffusion barrier of 0.23eV along the most favourable migration path. These results suggest that 1T-TaS_2 2D monolayer is a promising anode material for Li-ion batteries.

A1- 0054

Scrutinizing the interaction of DNA/RNA nucleobases with hexagonal-GeC monolayer: an ab-initio study.

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Abstract

The interaction between DNA nucleobases and two-dimensional materials is critical for advancing biosensing and their applications. In this study, we explore the adsorption properties of DNA nucleobases on a h-GeC monolayer using density functional theory (DFT). The adsorption energies and electronic properties are thoroughly analyzed to understand the nature of the interactions. Our primarily findings provide insights into the potential of h-GeC monolayer as platform for nucleic acid detection and bioelectronics. h-GeC is semiconductor and have direct band gap at K symmetry point with magnitude 2.09 eV. Here we calculate the interaction between h-GeC and Cytosine with electron correlation GGA. The predicted adsorption energy of cytosine onto h-GeC equal to 0.48 eV. The adsorbing of cytosine on h-GeC strongly influence electronic properties like energy band gap from 2.09 to 1.605. The strength of theoretical desorption time calculated for the Cytosine molecule 1.898×10^{-4} s at room temperature (300 K), it decreases at the higher temperature i.e. 1.509×10^{-6} s at 400 K.

A1- 0055

Enhanced room temperature NO_2 sensitivity of MoS_2 nano-flowers

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Abstract

In recent years, transition metal dichalcogenides (TMDs) have been investigated across multiple fields of science and technology. MoS_2, among the various TMDs has garnered significant interest of researchers due to its unique layered structure and remarkable optical and electrical properties. Thus, it has a wide range of applications including catalysis, gas sensing, energy storage, and hydrogen storage. In the present work, hydrothermal method with ammonium molybdate as a precursor has been used to produce two unique morphologies of MoS_2 viz. nanosheets and nanoflowers. Various characterization methods like X-ray diffraction (XRD), Scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy, and UV-Vis techniques ascertained the crystallographic structure, morphology, and band gap of the synthesized sample. The synthesized MoS_2 nanostructures showed a favorable response to 10 ppm NO_2 gas at room temperature with a response and recovery time of 68 and 3 seconds respectively. The detailed study confirms that the sensor exhibited an excellent sensitivity of more than 600% towards NO_2 gas at room temperature. Thus, adaptable morphology along with a tunable band gap of MoS_2 creates new opportunities in gas sensing technology.

A1- 0056

Ab-initio Investigation of the Gas Detection Mechanism of CCl_2O on Stanene

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Abstract

Two-dimensional (2D) allotropes like stanene exhibit significant potential for use in thin-film electronic devices. In this study, we investigate the gas sensing properties of toxic CCl_2O molecules adsorbed on single-layer stanene using first-principles density functional theory (DFT) calculations. The Perdew-Burke-Ernzerhof (PBE) form of the generalized gradient approximation (GGA) is employed as the exchange-correlation functional. Our predicted structural parameters, including lattice constant, bond length, bond angle, and buckling height of stanene, show excellent agreement with available data. Upon adsorption, the CCl_2O molecule stabilizes parallel to the stanene sheet at a vertical height of 3.5 Å. The band structure of stanene confirms its semimetallic nature, with no bandgap opening upon CCl_2O adsorption. Projected density of states (PDOS) analysis reveals that Sn-5p orbitals dominate both valence and conduction bands. Bader charge calculations show a transfer of 0.03 ē from the CCl_2O molecule to the stanene sheet, consistent with electron localization function (ELF) results, confirming physisorption. The calculated adsorption energy of -0.26 eV is in line with values reported for other gas molecules on similar substrates. Additionally, I-V characteristics suggest that CCl_2O adsorption induces back- scattering resistance. We feel that our theroetical predictions may help experimentalist working on developing future gas sensor technologies.

A1 -0057

Tunable Excitonic Emission in Monolayer p-MoS_2 Enabled by Charge Injection

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Abstract

Monolayer transition metal dichalcogenides (TMDs) play a pivotal role in optoelectronic applications due to their highly tunable optical properties, which can be precisely controlled through external factors such as strain, doping, and substrate interactions, enabling the development of highly efficient and customizable devices. In this study, we report tunable photoluminescence (PL) emission in monolayer p-type molybdenum disulfide (p-MoS_2) when fabricated on conductive substrates, including indium tin oxide (ITO), gold (Au), and few-layer graphene (FLG). This tunability in PL emission is enabled by charge transfer from the conductive substrates (ITO and Au) to p-MoS_2, facilitated by the difference in work function between them, resulting in enhanced PL emission in p-MoS_2. In contrast, at the p-MoS_2-FLG interface, charge transfer is likely inhibited due to the similarity in work function values between them, resulting in decreased PL emission. Upon cooling to liquid nitrogen temperature, further enhancement of PL emission is observed in p-MoS_2 on all substrates due to the suppression of phonon-assisted non-radiative transitions, reduced screening effects, and stronger Coulomb interactions, compared to room temperature emission. These results provide valuable insights into tuning the optical properties of 2D-TMDs, which are crucial for optimizing their performance in optoelectronic applications.

A1- 0058

Recovery of salt and conversion of dross waste into refractory material

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Abstract

Recycling and reusing industrial waste and by-products have become critically important in today's industry. Aluminium dross, classified as hazardous waste by the CPCB, requires careful recycling or safe disposal. This paper presents a clean and sustainable technology aimed at fully utilizing waste aluminium dross to achieve zero waste. We discuss the production of water treatment agents, such as poly aluminium chloride (PAC), through chemical leaching of the dross, and the use of the remaining dross in high alumina refractory castables.

In the current study, chemical leaching is used to extract the aluminum content from dross, which is approximately 15.42%. This aluminum is then processed to produce Poly Aluminum Chloride, a coagulant used in water treatment plants. The remaining dross is washed and its potential application in castables is explored. Additionally, the cold crushing strength of the treated dross was measured at 360/370 Kg/cm^{2}after being subjected to 110°C for 24 hours, which is comparable to the strength of castables made with bauxite.

The studies also revealed that waste aluminium dross can be used as alternative raw material in PAC preparation and alumina castable. This will help in utilization of aluminium dross in industries and help in reducing disposal to landfills.

Keywords: Aluminium dross, Poly Aluminium Chloride (PAC), Castable

A1- 0059

Influence of Yttrium ion doping on the structural, morphological and magnetic properties of cobalt ferrite nanoparticles

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Abstract

Here we report the synthesis of bare cobalt ferrite ($CoFe_2O4$) and Yttrium ($CoFe_{2-x}Y_xO_4$, x=0.05) ion incorporated cobalt ferrite using low temperature cost effective sol-gel self-ignition method. All the synthesis parameters were optimized to obtain fine particles with nanoscale dimensions. The monophase cubic spinel structure formation was confirmed through X-ray diffraction analysis. The unit cell parameter (a=b=c) was calculated through XRD data and was found to be 8.384 nm and 8.378 nm, respectively for bare cobalt ferrite and Yttrium doped cobalt ferrite. The crystallite size deduced from the Debye-Scherrer formula was found to be 24 nm and 18 nm. The structural analysis results shows strong influence of Yttrium ion doping. SEM images indicate the almost spherical nature of the grains with grain size 52 nm. The magnitude of saturation magnetization is decreased on doping of yttrium ion. All other magnetic parameters are also influenced by the yttrium ion doping. The observed magnetic behaviour was explained via Neil's model. The observed and calculated magnetic moment shows discrepancy in their values suggesting non collinear Behaviour.

Keywords: Cobalt ferrite, Yttrium ion doping, lattice constant, saturation magnetization, magneton number.

A1- 0060

Comparative Study of Powder X-Ray Diffraction Analyses of Titanium Dioxide (TiO_2) Nanoparticles

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Abstract

This paper describes the comparative study of Powder XRD Analyses of various samples of nanoparticle Titanium Dioxide (TiO_2) synthesised by the Sol-Gel method using Titanium (IV) isopropoxide Precursor. Titanium dioxide is relatively chemically inert and environmental friendly so it has been widely used in industry as a pigment and exists in the three phases like Anatase, Rutile and Brookite. X-ray diffraction (XRD) showed that prepared nanoparticles have pure anatase and anatase-rutile mixed structures. The prepared samples having different particles sizes (in nm) were observed at different ratio of precursor and the different calcination temperatures. This work has also analysed their various characters like specific surface area, dislocation density and morphology index.

A1- 0061

Cyclic Voltammetry Study of HRP enzyme immobilized over MoS_2 surface

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Abstract

The compound MoS_2 is a transition metal dichalcogenide (TMD) consisting of one molybdenum atom bound to two sulfur atoms. Its unique and diverse properties have challenged the superiority of graphene and other 2D materials. It thus has emerged as a front-runner in the development of small and portable electronic devices for a wide variety of applications. The negative charges carried by the MoS_2 nanosheets are used to immobilize horseradish peroxidase (HRP) through electrostatic attraction.
In this work, the HRP enzyme immobilized over the MoS_2 surface successfully. The results are confirmed by UV-Vis spectroscopy and Scanning Electron microscopy (SEM). And we have also studied their electrochemical behavior using the Cyclic Voltammetry technique over screen-printed electrodes. MoS_2 –HRP hybrid can be used for electrode modification for the investigation of different analytes in food, chemical, and pharmaceutical industries and other bio catalytic applications.

Keywords: TMD, molybdenum disulfide, 2D materials, HRP enzyme, nanosheets

A1- 0062

Structural and Optical behavior of conducting polymer based 'polymeric-inorganic' nanocomposites: Polyaniline/ZrO_2

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Abstract

In the present era, Nanoscience and Nanotechnology have attracted much attention at global level due to its ecofriendly solutions. It improves our quality of life by improving the fields of medicines and health care. In nanoscience, hybrid materials based on Polymer and nanoparticles are of great interest because of much improved properties of components compared to bare nanoparticles and polymer. In this article, we focused on the Structural and optical properties of Polyaniline-ZrO_2 nanocomposites. Zirconia is of great interest due to its very good properties as ceramics and when it is mixed with polyaniline it improves its structural, optical and electrical properties.

A1- 0063

Effect of calcination temperature on structural, morphological, optical properties and photocatalytic degradation behaviour of green synthesized ZnO nanoparticles by using fruit peels

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Abstract

Green ZnO nanoparticles synthesized via co-precipitation method by using orange peel extract were calcinated at different temperature (300ºC and 700ºC) followed by their structural, morphological, photocatalytic and optical properties characterization by using X-Ray Diffraction (XRD), Scanning Electron Microspocoy (SEM), UV-Visible and Fourier Transform Infrared (FTIR) Spectroscopy. The XRD spectra of zinc oxide (ZnO) nanoparticles indicate a shift of the characteristic XRD peak towards lower angles from 31.62º to 31.83º, 34.24º to 34.49º and 36.11º to 36.37º with calcination. The crystalline size of calcinated ZnO nanoparticles increases from 30.2 to 37.8 nm calculated from Scherrer's Method and from 33.5 to 45.5 nm measured from Rietveld Refinement method. UV-visible spectra show the absorption band at 468 nm and 671 nm respectively. Tauc plot has been drawn from the absorption spectra from UV data, the range of optical energy band gap of calcinated prepared samples lies between 3.67±0.07 to 3.35±0.02 eV. SEM and EDX confirm the presence of Zn and O in the prepared nanoparticles. The intensity of the absorption decreases steadily with increasing UV irradiation time for each annealed ZnO nanoparticle sample. The reduction in photocatalytic activity of the calcinated ZnO samples can be linked to the simultaneous decrease in both oxygen vacancies and surface-bound oxygen species.
Keywords: ZnO nanoparticles, FWHM, calcination and photocatalytic.

A1- 0064

Influence of silver nanoparticle on photolumines-cence of heat treated Ag-Er codoped tungsten tellurite glasses

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Abstract

The glasses of composition TeO 2 -WO3- Li2O-Er2O3 with AgNO3 (TWLEOAG) were prepared by the high-temperature melting method. Surface Plasmon resonance (SPR) bands are observed in the range 520-535 nm and 640-650nm of without erbium-doped glass by absorption spectrum. The TEM measurement reveals the presence of spherical AgNPs in this glass. The DSC has also been analyzed for the stability of transition temperature Tg and on set crystallization T0 of this glass system. The Raman spectrum revealed that TWLEOAG glasses were mainly formed by the [TeO4], {TeO3}, [WO4] and [WO6] units and [TeO4] units convert to [TeO3] units with the addition of WO 3 and Li2O content into tellurite glasses system. In particular TWLEOAG05 glass samples, heat-treated different time interval system reveal the enhancement in Raman peaks intensity with small shift in due to Ag nanoparticle. Also photoluminescence enhancement of red upconversion compare to green emission of TWLEOAG05 for different annealing duration has been observed under 808nm excitation. In this work optimum 0.5 mol% AgNP in TWEOAG glass would be useful for optical devices.

A1- 0065

Mn_3O_4/GO Nanocomposites for Advanced Electrochemical Biosensor for Detection of Fumonisin B_1

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Abstract

The presence of mycotoxins in food samples represents a significant safety risk due to their high toxicity and potential carcinogenic effects. This requires the development of highly sensitive and selective detection methods to ensure food safety. In this study, manganese dioxide (Mn_3O_4) nanoparticles were combined with graphene oxide (GO) to synthesize a nanocomposite aimed at enhancing the electrochemical performance of a biosensor for the detection of fumonisin B_1 (FB_1). A thin film of Mn_3O_4/GO nanocomposite on an indium tin oxide (ITO) substrate was prepared for an electrochemical biosensor. Antibodies specific for fumonisin B_1 (ab-FB_1) were then immobilized on the electrode using an electrophoretic deposition technique. To minimize non-specific binding, non-binding sites of ab-FB_1 on the immunoelectrode were blocked with bovine serum albumin (BSA). The final configuration of the biosensor was determined to be BSA/ab-FB_1/Mn_3O_4/GO/ITO, which enables efficient detection of fumonisin B_1 (FB_1) with increased specificity and sensitivity. The biosensor exhibited a sensitivity of 10.08 µA mL ng^{-1} cm^{-2}, demonstrating an impressive detection range from 1 pg mL^{-1} to 800 ng mL^{-1}. It achieved a limit of detection (LOD) of 0.195 pg mL^{-1}, highlighting its effectiveness in detecting low levels of FB1 in food samples. In addition, the recovery rate of BSA/ab-FB_1/Mn_3O_4/GO/ITO immunoelectrodes was evaluated using corn samples, yielding an impressive recovery of 98.91%. This high recovery rate indicates the reliability and efficiency of the biosensor for the detection of fumonisin B_1 (FB_1) in food matrices. The immunoelectrode demonstrated high reliability and reproducibility by continuous measurements on five electrodes.

A1- 0066

Optical and Magnetic Properties of Cobalt doped Gold Nano Clusters

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Abstract

The Cobalt (Co) doped gold nanoclusters have been synthesized using a low cost ligand-mediated wet chemical method. The scanning electron microscopic (SEM) analysis revealed the neural network morphology of the sample. From energy-dispersive X-ray spectroscopy, the concentration of Co dopant is found to be 0.18 %. The optical absorption properties of the doped and un-doped AuNCs have been studied in the presence of unpolarized and circular-polarized light as excitation sources. The circular dichroism (CD) study has confirmed the differing chirality features between undoped and Co-doped gold AuNCs. The CD indices of bare and Co-doped AuNCs show a strong band at 374.3 nm and 388.6 nm, and a weak band at 346.9 nm and 374.8 nm with contrasting magnitude of intensity respectively. This signifies the negative and positive chiral nature of un-doped and doped QDs. Fourier transform infrared (FTIR) spectroscopy data indicate a variety of absorption bands that correspond to typical stretching and/or bending vibrational modes. Magnetic measurements of the un-doped and doped QDs reveal the superparamagnetic (SPM) nature of the sample at 300k whereas ferromagnetic and antiferromagnetic behavior at 5 K respectively. These characteristics find numerous applications in Nano-photonics and Spintronics.

A1- 0067

Bimetallic Amine Functionalized Metal-Organic Framework Deposited on Graphene Oxide for Effectual Elimination of Cationic Dyes

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Abstract

Bimetallic Amine functionalized metal-organic frameworks/GO were prepared using a simple solvothermal process. X-ray diffraction (XRD), scanning electron microscopy (SEM), and Transmission Electron Microscopy (TEM) were used to characterize the as-prepared materials. The adsorption studies were conducted on Rhodamine B (RhB), and Malachite Green (MG) as a model organic pollutant. Compared to pure MOF, amine-functionalized bimetallic metal-organic frameworks with graphene oxide exhibit superior adsorption capacity. MOF/GO catalyst eliminates RhB and MG up to 99% in 120 min. This excellent adsorption is due to its unique micropore structure and its more negative zeta potential resulting from charge balancing for the protonation of $-NH_2$. Incorporating Ce(III) metal ions into bimetallic MOF plays an important role in adsorption because it increases the specific surface area and the number of adsorption sites and changes the surface charge of MOF channels. The addition of graphene oxide (GO) to the bimetallic metal-organic framework, greatly improves both the overall performance and dye adsorption capacity due to π-π interactions, electrostatic interactions, ionic bonding interaction, hydrogen bonding, and pore-filling mechanism. Langmuir adsorption isotherm and second-order kinetics fit well for the adsorption of both dyes. The prepared material would serve as a low-cost, environmentally friendly, and efficient catalyst for sequentially removing aquatic pollutants.

A1- 0068

Experimental and computational validation of Shell and Tube Heat Exchanger through α-Al_2O_3 based nanofluid

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Abstract

Shell and tube heat exchangers are widely used in various industries to transfer heat energy from a hot fluid to a carrier or cold fluid. Heat exchangers are categorized as either parallel or counterflow, depending on whether the hot and cold fluids flow in the same or opposite directions, respectively. To assess the effectiveness of a heat exchanger, two methods are commonly employed: The Log Mean Temperature Difference (LMTD) method and the ϵ-NTU method. Numerous previous studies have focused on enhancing the heat transfer performance of heat exchangers by using nanofluids, which are created by adding nanoparticles to a base fluid, such as water. In the present study, α-Al_2O_3 and γ-Al_2O_3 nanoparticles were successfully synthesized using the calcination process, and their structures were confirmed using X-Ray Diffraction (XRD) analysis. These nanoparticles were then used to create nanofluids with 0.1, 0.3, and 0.5 vol% of α-Al_2O_3 (alumina) nanoparticles in a 50:50 mixture of ethylene glycol (EG) and water as the base fluid. The prepared nanofluids were utilized as the hot fluid in a shell and tube heat exchanger to experimentally analyze changes in effectiveness and the overall heat transfer coefficient. The experimental results were also used to validate numerical calculations. Additionally, a 1 vol% sample was simulated numerically as the hot fluid. The results showed that the overall heat transfer coefficients for 0.1, 0.3, 0.5, and 1 vol% were 6.9%, 8.4%, 10.42%, and 15.9%, respectively. Similarly, the effectiveness of the heat exchanger was calculated as 4.4%, 6.36%, 8.5%, and 14.38%, respectively. Furthermore, the values of the Reynolds number, Prandtl number, and Nusselt number were found to exceed 45,200, 21, and 66, respectively, indicating turbulent flow, where convective heat transfer dominates over conductive heat transfer between the hot and cold fluids, and dynamic viscosity plays a more prominent role than kinematic viscosity.

A1- 0069

Design and evaluation of by hybrid Au-1D-photonic crystal based plasmonic biosensor

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Abstract

A hybrid gold (Au) layer and one dimensional photonic crystal (1D-PC) having periodic grapheme/PMMA based surface plasmon resonance (SPR) sensor with specific thickness of Au thin film and graphene layer has proposed better sensitivity in the Kretschmann configuration [1-2]. Sensitivity is not only parameter defined the performance of a biosensor; however resolution and Figure Of Merit (FOM) are equally important parameters for a biosensor [3]. These parameters are somehow depending upon the Full Width at Half Maxima (FWHM), where narrow and dip value of FWHM of the plasmonic biosensor gives better resolution and FOM. The narrow and dip value of the FWHM are found better resolution and FOM of the hybrid Au-1D-PC structure due to the propagation of non-radiative SPR and SEW waves i.e. the excitation of surface plasmon and surface waves. Hence, 1D-PC based plasmonic biosensor is designed based on hybrid Au-1D-PC, and evaluated reflectance of the hybrid Au-1D-PC structure with varying the thickness of Au film and number of the graphene layers by using simple Transfer Matrix Method (TMM) [4]. The calculated reflectance reveals that the biosensor based on 8 bilayers of grapheme/PMMA containing single layer graphene has to found better sensitivity in comparison to 6 bilayers of grapheme/MMA containing double graphene layers due to narrow and dip value of FWHM of the 8 bilayers of grapheme/PMMA containing single layer graphene.

Keywords: Photonic crystal, Gold hybrid graphene and PMMA plasmonic biosensor, Surface plasmon resonance (SPR).

A1- 0070

Structural and Microstructural Investigation on the Nanocrystalline Nd:Y_2O_3

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Abstract

In recent decades the nano crystalline high temperature ceramic material drags the interest of the researchers to explore its various structural, mechanical, electrical, magnetic, optical and thermal properties. One such metal oxide is Ytrrium Oxide (Y_2O_3) commonly termed as yttria which is a good host material, thermodynamically stable, have high-k dielectric constant and optically active material. In this present investigation the rare earth element (REE) Neodymium (Nd^{3+}) is used as the dopant. The nanocrystalline Nd:Y_2O_3 with 5% neodymium as dopant was synthesized by simple single step co-precipitation method and the synthesized sample was annealed at 750^o C to increase the crystallinity. The phase and structural analysis was performed using Powder X-ray Diffraction technique (PXRD) which shows that the synthesized sample were single phase in nature with Nd:Y_2O_3 crystallizing in cubic crystal system and the crystalline size was 9-13 nm for the samples annealed at 750^o C. The UV-Vis spectroscopic studies explain the optical parameters which confirm that the material is optically active. The SEM images reveal the surface morphology along with the shape of the particles and the elemental composition was confirmed to be 5% of Nd^{3+} dopant in Y_2O_3 host which was determined using EDAX analysis. The emission spectra obtained from fluorescence spectroscopy suggests that the emission and excitation wavelengths found between 400-950 nm. These preliminary results shows that the synthesized Nd:Y_2O_3 can be used as the contrasting agent in bioimaging, also the emission and excitation wavelengths suggests that it can be used in first biological window.

A1- 0071

Deciphering competing mechanism of Kitaev-Heisenberg-Gamma model in clusters

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Abstract

In this report discuss the static and dynamic properties of Kitaev spin-liquid system considering a Kitaev-Heisenberg-Gamma system which might be relevant to certain materials. We show that for antiferromagnetic Heisenberg coupling, the eigenstate becomes simultaneous eigenstate of total Hamiltonian as well Heisenberg part also. This happens for a range of paremeters and static correlation function develops a plateau in this range. For ferromagnetic Heisenberg interaction corelation function shows monotonous behavior. We briefly discuss specific heat, susceptibility and magnetization behavior and compare them with recent experiments. In the second part we discuss the Majorana dynamics and show how the gauge and matter Majorana fermions changes in time. We show that depending on the external magnetic field the gauge fermions can be stabilized to Kitaev limit and become weekly time dependent. We also discuss quantum speed limit and regular oscillations in the case when the ground state eigenstate become simultaneous eigenstate of Heisenberg interactions. We end with a outline how to extends our study to thermodynamic limit connecting with realistic experiments.

A1- 0072

PEG-coated ZnO:Er3+ upconverting nanoparticles for biomedical applications

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Abstract

Er3+ ion doped ZnO up-conversion nanoparticles were synthesized by using chemical co precipitation method. PEG (Polyethylene glycol) coating was done to make it hydrophilic and biocompatible. X ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), Field Emission Scanning Electron Microscopy (FESEM) and Raman spectroscopy characterizations were performed for the developed ZnO:Er3+ and ZnO:Er3+@PEG nanoparticles. UV-visible study shows an interesting absorption edges shifting due to the addition of PEG. The variation of PEG amount was systematically monitored. The upconversion emission study was carried out under 980 nm CW laser diode excitation. Energy level diagram has been represented to show the various radiative transitions originated from the Er3+ ions. Thermal conductivity measurement was done for the synthesized ZnO:Er3+ and ZnO:Er3+@PEG nanoparticles. A noticeable decrease of the thermal conductivity was reported on variation of the temperature upto ~400 K. highly aqueous soluble ZnO:Er3+@PEG nanoparticles are biocompatible and shows potential application in biomedical.

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Keywords: Upconversion, Chemical Co-precipitation, Thermal Conductivity, polyethylene glycol (PEG),

A1- 0073

Sol-Gel Derived ZnO: A Comprehensive Study of Synthesis and Properties

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Abstract

Zinc oxide (ZnO) nanoparticles have gained significant attention due to their exceptional properties, including their wide band gap, high chemical stability, and excellent optical and electrical characteristics. These properties make ZnO a promising material for a wide range of applications including optoelectronics, sensors, energy storage, and biomedical fields. Therefore, the objective of this study is to synthesize zinc oxide nanostructure using sol-gel method and characterize the nanomaterial. The structural, morphological and optical properties of the synthesized nanomaterial was analyzed using X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray (EDX) spectroscopy and Fourier transform infrared (FTIR) spectroscopy. XRD result spectrum displays mainly oxygen and zinc peaks, which indicate the crystallinity in nature as exhibited. The obtained ZnO nanoparticles are in the range of 20-22 nm calculated by Debye Scherrer method. SEM micrographs shows that synthesized ZnO have a sphere structure with good porosity. Result of EDX characterization shows that the ZnO nanoparticles has good purity.

A1- 0074

Reflection, transmission and absorption spectra of Te/PS multilayer structure with defect of metamaterial at terahertz region

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Abstract

The interaction of wave with matter defines the optical properties of periodic of one dimensional periodic structure (1DPS) of the materials. The optical properties like reflectance, transmittance and absorption spectra of one dimensional (1D) tellurium and polystyrene based symmetric and asymmetric periodic structure theoretically analyzed with defect of meta-material using the transfer matrix method (TMM). Reflectance, transmittance and absorption spectra are analyzed for symmetric structure found an enormous band gap which works as a broadband reflector and asymmetric structure shows the separated huge band gap in two parts. The defect of meta-material inserted in the tellurium and polystyrene based periodic structures are analyzed the broadband reflector, multichannel filter and sensor applications at terahertz region.

Keywords: Tellurium, Polystyrene, Meta-material, Photonic Crystal, Broadband multichannel filter and Sensor

A1-0075

Annealing study of silicon ion implanted Gallium Arsenide

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Semi insulating gallium arsenide samples of size 1 cm x 1 cm were implanted with low energy (100 keV) silicon ion beam for the fluences of 5 x 10^{15}, 1 x 10^{16}, 1 x 10^{17} ion cm^{-2} at low energy ion beam facility center in IUAC, New Delhi. Two sets of samples were prepared for each ion fluence. One set of samples were annealed in Furnace under N_2 ambient condition. The electrical property modification of silicon ion implanted (implanted for the fluences between 5 x 10^{15} and 1 x 10^{17} ion cm^{-2}) semi-insulating gallium arsenide sample before and after annealing (annealed for temperature up to 300K) was analyzed using and I-V measurement technique and Hall effect technique. I-V measurement study revealed increase in conductivity for silicon ion implanted gallium arsenide samples post annealing with same ion fluence sample. The Hall Effect study revealed increase in electron concentration post annealing with respect to same ion fluence sample.

Keywords: Silicon ion implantation, gallium arsenide, I-V measurement,

A1- 0076

Green Synthesis of Vibrant Plasmonic Nanoparticles using Calendula Officinalis extract as reducing and stabilizing Agent

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Abstract

Utilizing plant-based extracts, green synthesis provides an efficient, affordable, and environmentally friendly method to synthesize vibrant plasmonic NPs, minimizing ecological footprint. By eliminating hazardous chemicals, this biosynthetic method provides a safer, more environmentally responsible option for NP synthesis. This study demonstrates a novel, eco-friendly approach to synthesizing vibrant plasmonic nanoparticles (NPs) utilizing Calendula Officinalis (marigold) flower extract as a reducing and stabilizing agent. The Calendula Officinalis extract effectively reduced both gold and silver metal ions, resulting in the formation of uniformly sized, spherical NPs with remarkable plasmonic properties. Tuning the ratio of metal ion to extract concentration successfully synthesized the nanoparticles of different sizes as depicted by UV-Vis spectroscopy. The as-synthesized NPs displayed excellent stability and differential plasmonic signatures, making them promising candidates for applications in catalysis, sensing, and photovoltaics.

Keywords: Green synthesis, Plasmonic nanoparticles, Calendula Officinalis, Localized Surface Plasmon Resonance.

A1- 0077

Study of Gain Spectra in Optical fiber under Modulation Instability

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Abstaract

In this paper, we consider the phenomenon of modulation instability. Due to nonlinear phenomenon of self-phase modulation, the propagation of continuous wave beam is essentially unstable. For modulation instability, we plot various curves for gain spectra and find the maximum gain which shows the gain dependence on power, group velocity dispersion parameter and nonlinearity parameter.

Key words: modulation instability, gain spectra, dispersion, nonlinear

A1 -0078

Prediction of Thermophysical Properties of Nanomaterials: A Theoretical Study

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Abstract

The present study incorporates high pressure equations of state (EOSs) to study some thermophysical properties of nanomaterials. The thermophysical properties under study are pressure dependence of volume, pressure dependence of isothermal bulk modulus, Gruneisen Parameter at high pressure.

Keywords: High Pressure, Bulk Modulus, Gruneisen Parameter

A1- 0079

Graphene-Graphulerene Heterostructure: A Novel materials for High-Performance Capacitors

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Abstract

This study introduces a novel graphene-graphulerene heterostructure as a promising material for high-performance capacitors. Compared to pristine graphene, this heterostructure exhibits a significantly larger surface area and porosity, enhancing its energy storage capacity. While pristine graphulerene is a semiconductor with a bandgap of 0.92 eV, its integration with graphene effectively modifies its electronic properties, rendering it conductive as confirmed by band structure analysis. The unique combination of graphene's high conductivity and graphulerene's extended surface area and porosity presents a promising avenue for developing capacitors with exceptional performance characteristics.

A1- 0080

Investigation of Structural and Magnetic Properties of $Ba_{0.8}Y_{0.2}Fe_{10.3}Co_{1.7}O_{19}$ Nanoparticles

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Abstract

M-type barium hexaferrite, $Ba_{0.8}Y_{0.2}Fe_{10.3}Co_{1.7}O_{19}$ powder was synthesized using sol gel auto combustion method and heat treated at 850^0, 950^0, 1050^0 and 1150^0C. Effect of calcinations temperature has been studied using x-ray diffraction (XRD), Fourier transform infra-red (FTIR) spectroscopy and vibrating sample magnetometer (VSM). X diffraction (XRD) powder patterns of heat treated samples show the formation of M-type hexaferrite. The presence of two peaks at 427 $cm^{-1}$and 579 cm^{-1} in FTIR spectra gives the idea of the formation of M-type hexagonal ferrites .The M–H curve obtained from Vibrating Sample Magnetometer (VSM) was used to calculate saturation magnetization (MS), retentivity (Mr), squareness ration (SR) and coercivity (Hc). The maximum value of coercivity (2393Oe) is found at 850^0C. Coercivity is found to decrease with increases in temperature.

Keywords: Barium hexaferrite**,** magnetic properties, structural properties.

A1- 0081

Structural, Morphological, Compositional, Electrical and Optical Characterizations of Cuzns Thin Films Prepared Using Chemical Bath Deposition Method

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Abstract

Solar energy is remarkable due to its universal presence, affordability, abundant, and free high energy power output. The materials used to make solar cells are both non-hazardous and widely accessible on our planet. Here we report the structural, morphological, compositional, electrical and optical studies of the CuZnS thin film prepared using the chemical bath deposition method. *The pH of the precursor solution was 11.6. Samples were prepared by varying the time of deposition and temperature.* The methodologies adopted for the studies were *XRD [*Bruker Kappa Apex II*], SEM – EDAX [*Jeol 6390LA/ OXFORD XMX N], UV-Vis Spectrophotometry[JASCO V-670 UV-Vis NIR Spectrophotometer] and Hall effect measurement system [Ecopia HMS 3000s]. The parameters extracted from the electrical studies include Mobility, Sheet resistance, Resistivity, Conductivity, Average Hall coefficient, etc where these values set only for the corresponding thickness of the thin film. *The thickness measurement* of the thin film was done using Profilometer.

A1- 0082

Low temperature magnetic studies of $NdFeO_3$ synthesized by starch-assisted sol-gel combustion method

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Abstract

Single-phase neodymium orthoferrite ($NdFeO_3$) with an orthorhombic perovskite structure was synthesized using a starch-assisted sol-gel combustion method, free from garnet impurities. Magnetic analysis revealed that $NdFeO_3$ undergoes a transition from antiferromagnetic to paramagnetic behavior at Neel temperature of 650 K, indicating strong magnetic interactions between Fe^{3+} ions. Low-temperature studies further unveiled complex magnetic interactions involving Nd-Nd, Nd-Fe, Fe-Fe, and Fe-O-Fe couplings, which reflect the intricate magnetic dynamics, characteristic of rare-earth orthoferrites. The coercive field (H_C) of the air-grown sample was measured to be approximately 75 Oe, significantly lower than that of oxygen-grown nanocrystals, suggesting that differences in magnetic anisotropy arise from variations in the synthesis environment. Additionally, the temperature dependence of the magnetization followed Bloch's $T^{3/2}$ law, with a B-parameter of 2.60×10^{-5} $K^{-3/2}$, indicating the presence of spin-wave excitations. Sharp declines in coercivity were observed at 220 K and 580 K, likely due to changes in magnetic ordering. Above 580 K, the coercivity dropped sharply as antiferromagnetic interactions weakened, indicating a transition towards a more paramagnetic state.

A1- 0083

Effect of Plasmon Resonance of Metal Nitrides in Semiconductor Plasmonic Devices

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Abstract

The dipole-dipole interaction between Donor (D)–Acceptor (A) fluorophore pair leads to the Förster Resonance Energy Transfer (FRET) from donor to acceptor. This non-radiative transfer of energy has found applications in detecting protein folding and biosensors for clinical, pharmaceutical, toxicological, environmental monitoring and agri-food analysis. Majority of the traditional fluorophores used as D-A pairs are low-cost dies, identified by closely spaced broad absorption/emission spectra. Lately, QDs has emerged as versatile materials that can be used as both donors and acceptors in FRET provided absorption spectra of acceptor QD overlaps with the emission spectra of donor QD. The emergence of QDs based fluorophores is attributed to their high extinction coefficients as compared to organic dyes, broad excitation spectra, narrow emission spectra and large surface to volume ratio. As is well established, Localized Surface Plasmons of metallic nano system placed in the vicinity of QD fluorophores can greatly enhance FRET, and subsequently the performance of devices like LEDs, Solar Cells, Luminescent Solar Concentrators and Biosensors. In view of high bio compability, low intrinsic loss, low work function, high melting point etc. of ZrN and TiN, the role of ZrN/@SiO_2, TiN@SiO_2, ZrN/@TiO_2 and TiN@TiO_2 core-shell nanoparticles in modifying FRET parameters *e.g.,* FRET rate, FRET efficiency and Förster radius for CdSe QDs have been investigated. The optimized designs based on CdSe and Si QDs will be reported.

A1- 0084

Silver Glass Nanocomposites based UV Band Pass Filters

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Abstract

Glasses loaded with noble metal nanoparticles (Ag, Au, Cu) are considered as excellent candidates for the fabrication of ultrafast optical switches, optical sensors and waveguides which are of great importance in opto-electronic and photonic devices. In the present work silver glass nanocomposites were fabricated by Ag^+ - Na^+ ion-exchange method followed by 200 keV Ar^+ ion implantation at an oblique angle of 50^o with varying doses of $5x10^{15}$, $1x10^{16}$ and $5x10^{16}$ ions cm^{-2}. Thus fabricated nanocomposites were further characterized using field emission electron microscopy (FESEM) along with energy dispersive X-ray spectroscopy (EDAX), transmission electron microscopy (TEM) and UV-visible spectroscopy in transmission mode. The transmission spectra reveal that there is a narrow band in the UV region lying in a range of 340-360 nm for the nanocomposites which is absent in case of virgin glass and can be of significant importance from the perspective of UV based narrow band pass filters. When the dose of incident Ar^+ ions was increased from $5x10^{15}$ to $5x10^{16}$ ions cm^{-2} then transmission intensity decreased from 64.2 % to 53.2 %. Furthermore, the FWHM also showed a decrease from 62.4 nm to 47.9 nm for the nanocomposites with same doses.

Keywords: Silver glass nanocomposites, Ion implantation, UV band pass filters.

A1- 0085

One pot hydrothermal synthesis of WO_3 and its reduced graphene oxide nanocomposites for high-performance supercapacitor

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Abstract

Redox-active materials can store more energy than carbon-based electrode materials due to their various oxidation states[1]. Tungsten oxide-based nanomaterials has environmental friendliness, outstanding electrochemical stability, low cost, various crystalline phases and oxidation states (W^{2+}–W^{6+}) and chemical stability but comparatively less electrical conductivity as compared to carbon based materials . The combined materials with synergistic effects and integration of properties of each component can be widely used for high capacity storage devices[2]. In this study, a series of WO_3 /graphene nanocomposites with various weight ratios of tungsten oxide and reduced graphene oxide (rGO) are effectively synthesised using a simple one-pot hydrothermal method. Cyclic voltammetry, galvanostatic charge/discharge, and electrochemical impedance spectroscopy were used to examine the improvement in electrochemical supercapacitive capabilities from WO_3 to the various hybrids, depending on the concentration of GO injected. At a graphene oxide weight ratio of 0.2 wt % , a high rise in capacitance value of 494 F/g, surpassing the individual specific capacitance of rGO (71.11 F/g) and WO_3 (296 F/g) at a scan rate of 0.1V/s was demonstrated. This research work presents a novel method for attaining extraordinary charge storage contribution in crystalline metal oxides with minimum amount of GO.

A1- 0086

Numerical Optimization of TiN and ZrN Nanorods based Plasmonic Nanosystems for Enhanced Solar Absorption

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Abstract

The global cumulative photovoltaics (PV) installation already reached around 1600 GW and that of India around 89.4 GW. Moreover, the production growth rate of PVs is getting doubled every three years. Hence, the design and development of cost effective and efficient solar cells is the need of hour. Surface Plasmon (SP) mediated nanosystems are known to overcome the bottleneck of limited absorption in thin film solar cells characterized by typical thickness ranging between few nm to μm. In order to widen the list of plasmonic materials for photovoltaic applications, the present work considers Titanium Nitride (TiN) and Zirconium Nitride (ZrN) as plasmonic materials. Since they are known to show plasmonic response in UV-IR range, hence the possibility of significant overlap with solar spectra as required for PV applications. Their low cost, low dielectric loss, high melting point and fabrication compatibility put them at par if not ahead of noble metals (*e.g.,* Ag, Au, Cu, Pt, Pd *etc*.), the conventional plasmonic materials. Nanorod as well as core-shell nanorods based on above mentioned metal nitrides will be investigated and the optimization of solar absorption with respect to plasmonic material, rod length, core size, shell size and the embedding medium will be done. The performance of nitrides will be compared with that of gold (Au), one of the most widely used plasmonic material. Finally, nitrides nanorods based plasmonic designs optimized numerically for maximum overlap of plasmonic spectra with solar spectra will be reported.

Keywords: Photovoltaics, Light Absorption, Nanorods, PV, Titanium Nitride, Zirconium Nitride, Plasmonics, Nanostructures

A1- 0087

Melting temperature of nano Germanium-Ge, Tellurium-Te, Rhenium-Re, Osmium-Os and polonium-Po for different shape and size

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Abstract

In our present work, we are investing several nanosolids Viz. (Germanium-Ge, Tellurium-Te, Rhenium-Re, Osmium-Os and polonium-Po) with the aim of theoretically predicting their meting temperature at different shapes and sizes, by using the equation of W.H.Qi for calculating the melting temperature of nanosolids (Spherical nanosolids, nanowires and nanofilms).The equation established the relationship between the melting temperature of bulk material and their shapes and sizes. The size of nanosolids declines, the melting temperature of nanosolids also declines. Interestingly, our calculation reveals that the close alignment in the melting temperatures of spherical nanosolid, nanowire and nanofilms. By analyzing the calculated data, we have observed when the size is less than 5nm; their melting temperature demonstrates a significant reduction.

A1- 0088

Mexican-hat Band Structures in Bilayer Graphene

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Abstract

The electronic band structure of bilayer graphene (BG) is examined in this work. This study uses the tight-binding (TB) approximation method to investigate the impacts of bias voltage. To account this effect, the number of atoms per unit cell has been increased across the lattice. Applying bias voltage exposes an interesting Mexican hat-shaped pattern close to the K and K' points, as well as how this pattern changes with the number of atoms per unit cell.

A1- 0089

Low Ion Beam Irradiation-Induced Structural Modifications in GO-CNT-PANI Electrode Materials for Supercapacitor

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Abstract

This study investigates the structural changes in Graphene Oxide-Carbon Nanotubes-polyaniline (GO-CNT-PANI) spin-coated thin film samples induced by low-ion beam irradiation. The samples were irradiated with Argon (Ar) ions at energy of 10 keV, a current of 500 µA, and a fluence of 1×10^{16} ions/cm². Characterization techniques including X-ray diffraction (XRD) and scanning electron microscopy (SEM) were employed to analyse these changes. XRD analysis revealed a decrease in crystallinity post-irradiation. SEM images indicated morphological changes, with irradiated GO-CNT-PANI displaying a less damaged and more uniform surface structure. These findings suggest that GO-CNT-PANI maintains higher structural stability under low-ion beam irradiation, making it a promising candidate for durable and efficient supercapacitor Application.

A1- 0090

RESONANCE STUDY OF ALLIUM CEPA (ONION) EPIDERMAL CELL USING SPLIT RING RESONATOR AT 1 - 4GHz MICROWAVE FREQUENCIES

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Abstract

Microwave signal have various applications in biomedical science, including medical imaging, hyperthermia treatment, non-invasive glucose monitoring, remote patient monitoring, and tissue characterization. Microwave-based breast cancer detection has been proposed as a complementary approach to compensate for some drawbacks of existing breast cancer detection techniques recently. Microwave treatment methods are based on microwave sensors which are widely utilized in the field of medicine for non-invasive sensing, diagnostics, and therapy due to their harmless nature and ability to penetrate biological media. However, further technological advancements are necessary to fully harness the potential of microwave sensors in their design as the understanding the functionality of microwave sensors is crucial. Split Ring Resonator (SRR) is a commonly used sensor nowadays due to its ease of fabrication and utilization.

The efficiency SRR based microwave sensors depends on optimal position of the sensor, resonance frequency, material of the sensor, sampling size and activity of sample. In this study we optimized the position of the SRR in relation to the receiving antenna to get maximum resonance dip. The resonance frequencies of fabricated SRRs are confined in a frequency range of 1-4GHz for proposing its application in biomedical diagnosis. As the efficiency of sensors depends upon the material used for the fabrication of the SRRs, copper and silver based SRRs are used for the studies. Additionally, the minimum sample size that can be analyzed by the SRR sensor is an inevitable parameter for using SRR in sensor applications. Different dimensions of Allium Cepa (Onion) samples are used to optimize the sample size. Resonance studies of living and dying cells are also carried out in order to understand the biological condition of the cells. Beyond biomedical applications, microwave sensors have a wide range of potential uses, including the analysis of food adulteration and the differentiation and analysis of various chemical compounds with high accuracy and precision in the future

A1- 0091

Exploring the SnO_2 Nanoparticles at different temperatures prepared by chemical co-precipitation technique

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Abstract

Pure SnO2 Nanoparticles were synthesized by chemical co-precipitation technique at different temperatures. Using XRD, FTIR and UV- Vis spectroscopy the structural and optical analysis of prepared samples have been done. The XRD pattern of SnO_2 exhibited sharp peaks which indicated good nanostructures. The average crystalline sizes of prepared samples were found in the range of 11.143 - 16.837 nm. The IR spectrum displays different vibration peaks. The energy band gap of SnO_2 was calculated using Tauc's plot and values of Eg are 3.8, 3.7 & 3.6 eV. Prepared SnO2 are shown to have good nanostructures and optical properties that indicate great suitability for optoelectronic and large band gap engineering applications.

Keywords: SnO2 Nanoparticles, XRD, FTIR, UV-vis and Tauc plot

A1- 0092

Structural, electrical, magnetic and electrochemical studies of Copper substituted lithium ferrite prepared by Ceramic method using high energy ball milling.

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Abstract

Copper substituted lithium ferrite of the compositional formula $Li_{0.5-0.5x}Cu_xFe_{2.5-0.5x}O_4$(x=0.0, 0.1, 0.2, 0.3, 0.4, 0.5) was synthesized via the ceramic method using high energy ball milling. The prepared samples were calcined at 900°C for 3h and sintered at 1000°C for 2h. The sintered samples were used for various characterizations. Structural and phase analysis were done using the X-ray Diffraction (XRD) and FTIR data. The XRD spectral analysis confirmed the single cubic phase with spinel structure. The structural parameters such as crystallite size and lattice constant of the samples were calculated using XRD data and studied for the varying copper content. Electrical measurements were carried out at room temperature in the frequency range 500Hz to 5MHz using LCR meter. VSM measurements were carried out to study the magnetic properties. The magnetic parameters like saturation magnetization, coercivity, remanence and remanence ratio were studied with variations of the copper concentration. Electrochemical properties of undoped and copper doped lithium ferrite electrodes have been investigated by cyclic voltammetry in 2M KOH electrolyte. The results obtained have been discussed and reported in the paper.

Keywords: lithium ferrite, XRD, FTIR, SEM, VSM, electrochemical properties

A1- 0093

Study of Effect of Calcinations Temperature on Structural and Magnetic Properties of $MnO_{2-\lambda}$ Nano-crystallines

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Abstract

The today researchers are interested in studying nano-scale particulates as a result of their enhanced Physico-chemical and biological traits. Nano-particulates have significant properties at nano scale because of high surface to volume ratio and quantum size effect. The metal oxide nanoparticulates of MnO_2 have enhanced properties in the field of Energy harvesting, defence and medical etc. In the current work, pure MnO_2 nanoparticulates were prepared via a microwave irradiated chemical co precipitation protocol. The samples were further calcined at 200ºC, 400ºC, 600ºC and 800º Celsius for fixed duration 2hrs.The calcined samples were scanned through XRD, FTIR, FESEM, and VSM tools to examined the respective changes occurred with rise of calcinations temperature. The XRD results revels that MnO_2 nano-particulates were formed with different phase α- MnO_2,β- MnO_2,δ- MnO_2 crystal structures and phase transformation occurred with rise of temperature. The grain size of nanoparticulates were calculated by use of Debye Scherer estimation and crystalline size 27.47nm, 29.68nm, 32.80nm and 36.14 nm pattern shows that crystallite size increases with increase in calcinations temperature. The IR sharp peaks inspected at 450 cm, 424cm^{-1}, respectively and were attributed by O-Mn-O molecular vibration and supports the XRD results of studies. The Transmission electron microscopic image of samples shows that 2D nanofleck like structure with average grain size 37nm. The VSM characteristic of calcined samples concluded that saturation magnetization gradually decreases with increase of calcinations temperature and all substances were ferromagnetic in behavior. The materials have recommended applications as electromagnet formation.

Keywords: MnO_2 nanoparticulates, X-Rays Diffraction, FTIR, HRTEM and VSM tools.

A1- 0095

Studies on structural characterization, electrical, magnetic and electrochemical properties of nickel-substituted Co-Zn ferrite synthesized via ball milling Technique.

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Abstract

Nickel substituted Cobalt Zinc Ferrite with compositional formula $Co_{0.8-x}Zn_{0.2}Ni_xFe_2O_4$ (x=0.0, 0.05, 0.1, 0.15, 0.2, 0.25) were synthesized via conventional ceramic method utilizing ball milling technique. The synthesized ferrite underwent calcination at 900^0C for 3h and sintered at 1100^0C for 3h. Structural analysis through X-ray diffraction (XRD) confirmed the formation of a single-phase cubic spinel structure in all prepared samples. From the XRD data, structural parameters including lattice constant, crystallite size, and X-ray density were determined. FTIR was employed to examine the functional groups present, while scanning electron microscopy (SEM) provided detailed insights into the morphology, revealing grain size and grain distribution characteristics. The frequency dependence of the electrical properties was studied using an impedance analyzer and the dispersion behavior has been observed. Magnetic properties of the samples were explored using a vibrating sample magnetometer (VSM), and their electrochemical behavior was systematically analyzed through cyclic voltammetry in 2M KOH electrolyte, comparing both undoped and nickel-doped Cobalt Zinc ferrites. The findings of this study have been comprehensively discussed in the paper.

Keywords: Nickel substituted cobalt zinc ferrite, XRD, SEM, VSM, Electrochemical properties.

A1- 0096

Impact of Nitrogen Content on the Anti-Reflective Characteristics of *a*-SiNx:H thin Films

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Abstract

Amorphous hydrogenated silicon nitride (*a*-SiNx:H) films with varying stoichiometry were deposited on Si substrates using the Plasma Enhanced Chemical Vapour Deposition (PECVD) method. The precursor gas flow rates of SiH4 (4% in Ar) and NH3 were adjusted to obtain different film compositions. The refractive index of the as-deposited films, measured using single wavelength null ellipsometry at 628 nm, ranged from 1.54 to 2.56, with stoichiometry (x =[N]/[Si]) varying from 0.25 to 1.48. Photoluminescence (PL) spectra, recorded at room temperature with a 325 nm excitation source, showed a systematic red shift as the nitrogen content increased. This red shift is attributed to the increased presence of nitrogen dangling bonds in nitrogen-rich a-SiNx:H films. UV-Vis spectroscopy reflectance measurements, fitted with Finite-Difference Time-Domain (FDTD) simulations in Lumerical software, showed an excellent agreement with the experimental data. Films with a stoichiometry of x = 0.56 exhibited the lowest average reflectance (~ 19.06%), indicating their potential for photovoltaic applications. These results highlight the influence of nitrogen content on optical properties and the suitability of a-SiNx:H films for optoelectronic devices.

A1- 0097

Recent Development on V_2O_5 Gas Sensors: A Review

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Abstract

Vanadium pentoxide (V_2O_5) being a noteworthy transition metal oxide within the domain of chemical gas sensing, energy storage, catalysis, electronics, biomedicine, etc. offers high oxidation state, thermal stability, electrical conductivity, layered structure, excellent catalytic and optical properties. In the field of gas sensing, fabrication of a suitable responsive and selective gas sensing device the sensing material needs a significant surface-to-volume ratio for performance of absorbance of target gas on the surface-active material. From start to finish a variety of procedure frameworks have been encountered for fabrication [1] of a gas sensing device which includes direct oxidation, sol-gel method, co-precipitation method, chemical vapour deposition (CVD), template assisted method, electrochemical deposition, spray pyrolysis and hydrothermal synthesis namely. Agreeing to conditions for a suitable gas sensing material V_2O_5 lays groundwork for its different morphological structures as a result of having good stoichiometry and abundance of synthesis techniques which lead to development of desired nanostructures [2]. Depending upon factors such as morphology of sensing material, gas absorption rate, and temperature of operation gas sensing device selectivity, sensitivity and response can vary. For concise study of target material-based sensors different calculations are done to dive deeper response and recovery rate are analysed for a variety of gases for distinguished concentration and variety of temperatures. Here in this study, we aim to review the changes and modifications done on V_2O_5 gas sensors in recent times and summarize its impact, mechanism and applications as V_2O_5 is emerging as a suitable material for gas sensing processes due to its stability, low operational temperature, modifiable properties, and most importantly environmental compatibility.

A1- 0098

Optimization and Characterization of SnSe Nanoparticle

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Abstract

IV-VI group binary chalcogenides have unique electronic structure, coupled with tunable bandgaps, make them promising candidates for photovoltaic devices, thermoelectric applications, and infrared detectors. SnSe is a promising semiconductor candidate due to its lower toxicity and wide direct band gap of 2.96 eV. It possesses a layered structure where the layers interact with each other through Van-der Waals forces. This layered structure also offers potential sites for interaction. SnSe nanomaterial have been synthesized via cost effective simple solvothermal method. The solvothermal method is a chemical synthesis technique used to produce materials with conditions of high temperature and pressure in a solvent medium. This method is particularly useful for synthesizing nanomaterials, crystals, and complex compounds. This method offers several advantages over other techniques including precise control over particle size, morphology, versatility, scalability and crystallinity of the synthesized materials. The crystal structure and morphology of SnSe nanostructure were characterized using X-ray diffractometer and field emission scanning electron microscopy techniques respectively. The purity and optical properties of synthesized materials using EDX, UV- Vis and PL spectroscopic techniques respectively. The vibrational properties of synthesized SnSe sample were investigated using FTIR technique in the range of 500-4000 cm^{-1}. EDX confirmed that the formed material composition is SnSe also confirmed by the XRD pattern. The SEM micrographs of synthesized sample confirmed the formation of nanoparticles along with layers type structure.

A1-0099

Thermal transport through one dimensional trimer chain

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Abstract

The main challenge of the Nano scale devices is to manage the heat/phonon transfer through the devices. With this, the main aim of this study is to investigate the possibilities of enhance the control over the phonon propagation by changing the regular arrangement of different mass material. The focus of this paper is on the different one-dimensional trimer chain. Three layers of different materials, A, B, and C are considered and connected in series. For constructing a trimer model, the block ABC is then repeated to get long chain. This forms a periodic arrangement of layers having a period of layers ABC. Each layer has total 20 oscillators so that one period of ABC has total 60 oscillators. For the present simulation experiments, total four blocks of ABC are considered. Hence, the total length of a trimmer becomes four periods and the total number of oscillators in the trimmer chain is thus 60 x 4 = 240. The mass of each oscillator in layers A, B and C are MA=1.0, MB=0.5 and MC=1.5, respectively. In the course of present work, the thermal conductivity and heat flux of six types of trimmer chain viz; ABC, ACB, BAC, BCA, CAB, CBA are investigated, where a block is prepared by various series connections of material A, material B and material C. This study gives us the idea about the geometry dependent thermal transport in the trimmer chain

A1- 0100

Effect of Swift Heavy Ions Irradiation on Magnetic Anisotropy and Electron Paramagnetic Resonance studies of Ga-In substituted Strontium Hexaferrites

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Abstract

50 MeV Li^{3+} ion beam irradiation effects with respect to different fluence values on magnetic properties of single crystals of composition $SrGa_xIn_yFe_{12-(x+y)}O_{19}$ (x =0, 5, 7, 9; y = 0, 0.8, 1.3, 1.0) are studied using vibrating sample magnetometer (VSM) and EPR spectroscopy. Hexagonal ferrites ($SrFe_{12}O_{19}$) are widely known as technologically important materials having number of applications in electronic and/or magnetic devices. Considerable amount of work has been carried out to modify the properties of ferrites by different methods. Swift heavy ion irradiation is one of the effective tools for the modification of the properties of ferrites as ion bombardment may cause the modification or can improve certain properties of materials. The partial substitution of Fe^{3+} by non-magnetic ions like Gallium and Indium in Strontium hexaferrite has shown to be an effective method to tailor anisotropy for many novel microwave applications. Some basic studies have revealed that this substitution leads to unusual interactions among the magnetic sublattices of the ferrite.

In the present study, 50 MeV Li^{3+} ion irradiation decreases the value of magnetization with respect to the pristine one but the value of M_s increases in irradiated crystals with increase in the fluence value. The increase in magnetization with increase in fluence value is observed in Pure $SrFe_{12}O_{19}$ as well as $Ga_5In_{0.8}$ substituted Sr – hexaferrite. The value of anisotropy field (H_a) increases on irradiation which further decreases with increase in fluence value in both the crystals. Whereas the value of anisotropy constant (K_1) decreases on irradiation and increases with increase in fluence values in irradiated crystals. This increase in the value of magnetization and anisotropy field on irradiation may be explained due to appearance of new Fe^{3+} ions in amorphous phases of irradiated crystals, with a coordination number of five [36] i.e., 2b site which is mainly responsible for the anisotropy in M – type hexaferrites. Irradiation of both the crystals i.e., Pure $SrFe_{12}O_{19}$ as well as $Ga_5In_{0.8}$ substituted Sr – hexaferrite at different fluence values does not affect the value of curie temperature. Their ferromagnetic resonance spectra were also measured in the X-band (9.4 GHz), at room temperature. A broad resonance signal is observed in pure Sr-hexaferrite. This signal is typical of an ordered ferro- or ferrimagnetic phase. With the Ga-In substitution, this signal splits into two resonance lines exhibiting a progressive splitting into two peaks for substituted compositions to finally coalesce again into a single (paramagnetic) narrow peak at higher substitutions. These results are interpreted in terms of a substitution of Fe^{3+} by Ga^{3+} and In^{3+} ions in the 4 fvi and 2b sublattices; the diamagnetic cations disrupt the superexchange interactions and produce a splitting of the 12k sublattice (which interacts directly with the 4 fvi sublattice) into two sublattices with different canting angles, and different thermal dependence.

Keyword: Irradiation. Magnetization, Anisotropy Field, Magnetic anisotropy, Curie temperature

A1- 0101

Structural, Optical, and Transport properties of CZTS Semiconductor Nanoparticles Synthesized via Hydrothermal Route

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Abstract

Quaternary compounds such as chalcogenides composed of earth abundant and non-toxic elements have gained tremendous interest in photovoltaics. Cu, Zn, Sn, and S (CZTS) semiconducting materials find their potential applications in renewable energy sectors particularly in solar cells. Moreover, wide band-gap semiconductor nanoparticles prepared from group I-VI elements have attracted potential applications in the emerging energy alternatives. The band gap of these materials can be tuned with control over their particle size. Hence, an efficient synthesis route is required for precise control over particle size, morphology, and high crystallinity. Here, we report a synthesis of CZTS nanoparticles using the hydrothermal method. The developed nanoparticles were characterized using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and Scanning Electron Microscopy (SEM) for analyzing their structural properties and surface morphology. UV-visible spectroscopy was employed to obtain their optical properties. Thermal stability and related phase transition were studied using thermal analysis through thermogravimetric analysis (TGA) and Differential thermal analysis (DTA). The transport properties were studied using Hall Effect measurements. The derived CZTS nanoparticles show striking properties, making it a viable material for pertinent applications including photovoltaics and other optoelectronic devices.

A1-0102

Effect of precursor solution on the properties of ceria nanoparticles prepared by co-precipitation method

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Abstract

In this paper, the nanoparticles of cerium oxide were prepared by versatile co-precipitation technique. The effect of precursor on the structural and optical properties were analysed using XRD, UV-Vis absorption, Photoluminescence and FTIR technique. The formation of cubic fluorite structure was confirmed by XRD studies. The size of nanoparticles are so obtained were about 12nm. The marginal changes in the band gap were observed. The presence of Ce-O Stretching bands in FTIR confirms the formation of cerium oxide nanoparticles. The emission spectra obtained from photoluminescence technique gives violet and blue emission.

A1- 0103

Effect of annealing on defect formations in ZnO nanoparticles

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Abstract

This study reports effect of annealing on the structural, defect formation and optical properties of ZnO nanoparticles (NPs) synthesized using self combustion reactions. For investigating the effect of annealing, one part was kept as-synthesized and other two were annealed at 450ºC & 700ºC (referred as ZCA, ZCA450 and ZCA700). Rietveld refinement of XRD patterns confirmed phase pure ZCA, ZCA450 & ZCA700 in the wurtzite type hexagonal structure and monotonic increment in the unit cell volume and mean crystallite size with annealing temperature (AT). Further, observation of three characteristic $2E_{2H}$-$2E_{2L}$, E_2 (high) and E_1 (LO) Raman modes validated hexagonal symmetry of these samples. Blue shifting in the E_2 (high) and E_1 (LO) modes and red shifting in the $2E_{2H}$-$2E_{2L}$ mode. ESR analysis inferred formation of oxygen and zinc vacancies on the surface of ZnO NPs along with annihilation of surface defects with increasing AT. UV–visible-NIR spectra showed considerable absorption of light below 500 nm by these ZnO NPs with maxima in the blue region in the ZnO NPs. The obtained band gap E_g = 2.74 eV for ZCA NPs is found higher than E_g = 2.50 eV for ZCA450 and E_g = 2.68 eV for ZCA700. Notably, these E_g values are considerably lower than the reported values. These ZnO NPs seems to be useful for making UV & blue light protection layer and UV absorber for sunscreen lotion etc.

A1- 0104

Stability Analysis of Plasmonic Nanoparticles for Sustainable Applications

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Abstract

The distinctive plasmonic responses of noble metal nanoparticles in interaction with electromagnetic radiation have attracted a great deal of attention from researchers. Plasmonic nanomaterials (P-NMs) are remarkable for their optical, mechanical, and catalytic properties, making them highly valued in various applications such as sensing, disease treatment, and energy transfer and conversion. The research of P-NMs has gained popularity in recent decades, with an emphasis on their synthesis, characteristics, and wide range of uses. Effective stabilizing techniques are necessary to preserve desired performance since the plasmonic characteristics of these nanoparticles are complicated and related to size. Physical and chemical characteristics can be considerably changed by even small changes in particle size, which can have a substantial impact on total applicability. Consequently, in order to guarantee stability and maximize performance in a variety of devices and applications, we want a easy and simple technique as well as sensitive particle size monitoring. Different methods are used to check the stability of P-NPs(e.g. SLS, DLS,AFM,SEM,TEM etc.).SLS(Static Light Scattering) is very simple method, for tracking particle size. This article provide a stability study of plasmonic NP using SLS(static light scattering)method. The results are compared with another technique (e.g. SEM, TEM, UV-vis spectroscopy).

A1- 0105

Thermoluminescent Behaviour of $LiMgPO_4:Eu^{3+}$ for Dosimetric Applications

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Abstract

In this study, $LiMgPO_4:Eu^{3+}$ phosphor was synthesized via a single-step solid-state reaction method, and its thermoluminescence response against gamma ray exposure was investigated. From the personnel dosimetry point of view, tissue-equivalent material is highly desirable. The effective atomic number (Zeff) of the synthesized $LiMgPO_4:Eu^{3+}$ was analyzed to be 10.22, almost approximating the biological tissues. X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM) and Fourier-transform infrared spectroscopy (FTIR) technique were instrumented to characterise the sample in terms of its crystalline structure, particle surface and functional groups, thereby affirming the incorporation of Europium (Eu) within. Moreover, we also studied the thermoluminescence (TL) characteristics of the $LiMgPO_4:Eu^{3+}$ powder. The TL response was evaluated after exposure to gamma radiation doses ranging from 10 Gy to 10 kGy, and the measurements confirmed that the response was dose-dependent. The studied samples possess various levels of dopants, with a concentration range of 0.1 – 0.5%. In order to study thermoluminescence, several features were examined using Chen's peak technique, which is a foremost rise technique. It was clear for this material after studying the linearity of the different dopant concentrations produced for gamma rays that $LiMgPO_4:Eu^{3+}$ holds much potential to be used in gamma-ray dosimetry as a reliable means of radiation detection.

A1- 0106

Synthesis and characterization of surface modified metal/ metal oxide (Ni/NiO) core shell nanoparticles

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Abstract

Among various core shell nanoparticles, metal-metal oxide core-shell (M-MO) nanoparticles have gained wider interests due to their unique optical, electrical, and magnetic properties and finds pertinent applications in the field of electrocatalysis, photocatalysis, magnetic and electrical devices, sensors, electrode materials in supercapacitors, drug delivery, and bioimagining. The control over surface morphology and the surface functionalization is a major challenge for exploring wider range of applications, specifically in drug delivery and catalysis. Various efforts are being made towards development of the process providing tunability over core-shell materials (organic and inorganic), shape and size of such M-MO nanoparticles. Here, we report synthesis of Ni: NiO nanoparticles using microwave assisted sol-gel type chemical process. The reported process permits precise control over the morphology and the surface group functionalization with and without graphitic type carbon layer over the surface. The structural, compositional, and optical properties of the derived Ni:NiO nanoparticles were examined using X-ray diffractogram (XRD), Raman spectroscopy, and X-ray photoelectron spectroscopy (XPS).

A1- 0108

Effect of Nitrogen content on the Anti-reflection properties of a-SiNx: H thin films

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Abstract

Silicon nitride has been a material used in variety of applications ranging from good dielectric material to solar cells [1–3]. The ability to adjust the stoichiometry across a broad spectrum ranging from Si rich to N rich, provide the versatility to *a*-SiN*x*:H thin films, for diverse applications [4]. In present work we explore the effect of stoichiometry on the anti-reflection properties of *a*-SiNx:H thin films. *a*-SiNx:H films of different stoichiometry were grown on Si substrate using plasma enhanced-CVD method by varying the ratio of precursor gases SiH4 (4% in Ar) and NH3. Stoichiometry (*x*=[N]/[Si]) ranging from 0.25 to 1.48 corresponding to refractive index from 1.54 to 2.56 of as-deposited thin films, were calculated using single wavelength null ellipsometry operating at 628 nm. Photoluminescence spectra of thin films were recorded at room temperature using excitation source of wavelength 325 nm. A systematic red shift in the overall luminescence is observed with increasing N-content in thin films i.e. from *x*=0.25 to 1.48. This red shift is caused by an abundance of N dangling bonds in the N-rich *a*-SiNx:H thin film [5]. The reflectance properties were analysed using UV-Vis spectroscopy in 400-900 nm wavelength range, the effect of stoichiometry is observed. Films with *x*=1.48, 0.95 i.e. higher N content, show a lower reflection in higher wavelength but a higher reflection in lower wavelength region in comparison to thin films with higher Si content (stoichiometry, *x*= 0.55, 0.25). Further, to affirm the effect of stoichiometry on the properties of thin films FDTD simulations were employed to obtain the reflectance spectra using Lumerical software. The simulation results were found to be in good agreement with experimental results, establishing the stoichiometry dependence of reflectance. The ability to tune optical properties of *a*-SiNx:H films with stoichiometry, propose these thin films as the potential candidate for photovoltaic applications.

**Equal contribution* a *During the execution of this work the author was at the Department of Physics, Indian Institute of Technology Delhi.*

A1- 0109

Transport Properties of Bismuth Telluride and MoS_2 Composites

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Abstract

Molybdenum disulfide (MoS_2) is belonging to a class of transition metal dichalcogenide (TMD) compounds with layered structure. In this paper, we have synthesized MoS_2 by ball milling followed by sulfurization process. This synthesis method is simple and reliable to prepare the nano/micro particles of MoS_2. The composite of Bi_2Te_3 and MoS_2 materials prepared by varying MoS_2 concentration in weight percent ratio of 2%, 4% and 10 % and followed by mechanical alloying and vacuum hot press sintering technique. The structural analysis and thermoelectric properties of bulk composites were investigated. The XRD pattern of molybdenum sulfide showed phase formation and strengthened diffraction peaks are indicating improved crystallinity in MoS_2 due to annealing. Morphology of the composites shows the MoS_2 homogenously and randomly distributed in composite samples. The electrical resistivity decreased with increasing temperature indicating semiconducting character of composites. The Seebeck-coefficient as a function of temperature confirms the n-type nature of composites.

A1-0110

Investigating the Electrochemical Properties of SSCF Cathode in IT-SOFC Applications

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Abstract

This study explores the electrochemical properties of $Sm_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ (SSCF) cathodes for Intermediate Temperature Solid Oxide Fuel Cells (IT-SOFCs). Utilizing a combination of electrochemical impedance spectroscopy (EIS), we evaluated the performance characteristics of SSCF materials under varying temperatures and operating conditions. Our findings reveal that the SSCF cathodes exhibit high ionic conductivity, significantly enhancing their performance in IT-SOFCs. Analysis of electrochemical impedance data indicates low polarization resistance, suggesting efficient charge transfer mechanisms at the cathode-electrolyte interface. The results highlight the potential of SSCF as a viable cathode material, offering improved performance metrics that may advance the operational efficiency and durability of IT-SOFCs. This research provides critical insights into optimizing SSCF cathode formulations, paving the way for their application in next-generation fuel cell systems aimed at sustainable energy solutions.

Keywords: SSCF cathode material, Electrochemical Impedance Spectroscopy

A1- 0111

Rietveld Refinement Investigations of SSCF Cathode Characteristics for Enhanced IT-SOFC Performance

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Abstract

This study investigates the structural characteristics of $Sm_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ (SSCF) cathode materials through Rietveld refinement techniques to enhance the performance of intermediate-temperature solid Oxide Fuel Cells (IT-SOFCs). The SSCF materials were synthesized and characterized using X-ray diffraction (XRD) to identify phase purity and crystallographic properties. Rietveld refinement analysis provided detailed insights into the material's unit cell parameters, atomic positions, and thermal vibrations, elucidating the relationships between microstructural features and electrochemical performance. The implications of these findings are significant, as improved cathode performance directly correlates with the overall efficiency and durability of IT-SOFC systems. Our results highlight SSCF cathode's potential in advancing IT-SOFC technology's practicality for clean and sustainable energy applications.

Keywords: SSCF cathode material, XRD, Rietveld refinement

A1- 0112

Study of Vanadium Pentoxide (V_2O_5) Nanostructured Thin Films

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Abstract

In this study, we examine the effect of growth temperature on the structural and optical properties of vanadium pentoxide (V_2O_5) nanostructured thin films. The films were deposited with constant deposition duration of 45 minutes, while the growth temperature was varied at 350°C, 450°C, 550°C, and 650°C. The structural properties of the films were characterized using X-ray Diffraction (XRD), Raman spectroscopy, and Scanning Electron Microscopy (SEM), while X-ray Photoelectron Spectroscopy (XPS) was employed to analyze their chemical composition. XRD and Raman results revealed temperature-induced changes in crystallinity and phase transitions in the V_2O_5 films, with higher temperatures promoting more crystalline phases. SEM analysis showed significant changes in surface morphology with increasing growth temperature, indicating enhanced grain growth and particle coalescence. XPS confirmed the oxidation state and chemical composition of the films. The optical properties were studied using UV-Vis spectroscopy, where we observed a shift in reflectance and optical band gap with the variation in temperature. This research provides valuable insights into tailoring the structural and optical properties of V_2O_5 thin films through temperature control, with potential applications in optoelectronics and energy storage devices.

A1- 0113

Modifications Induced in the Structural, Optical, and Photocatalytic Properties of Cu and Mo co-doped $BiVO_4$

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Abstract

Comprehensive experiments were conducted to investigate the effects of Cu and Mo co-doping on the photocatalytic performance of bismuth vanadate ($BiVO_4$) nanoparticles. In this study, $BiVO_4$ nanoparticles were synthesized via the sol-gel method and characterized using X-ray diffraction (XRD), Raman spectroscopy, PL spectroscopy, UV-Vis spectroscopy, Synchrotron Soft XAS and field-emission scanning electron microscopy (FE-SEM). The XRD patterns and Raman spectra confirmed the crystalline nature of the material and its monoclinic scheelite phase. Morphological analysis using FE-SEM revealed the formation of homogeneous, spherical-shaped particles with sizes ranging from approximately 180 to 200 nm. Synchrotron-based soft X-ray absorption spectroscopy (XAS) provided detailed insights into the electronic structure, particularly the hybridization between vanadium (V) and oxygen (O) atoms. Photoluminescence (PL) spectroscopy was employed to examine charge recombination rates, demonstrating a significant enhancement in photocatalytic performance due to the presence of oxygen vacancies. Furthermore, the co-doping of $BiVO_4$ with Cu and Mo significantly improved its photocatalytic behavior compared to pristine $BiVO_4$.

A1-0114

Conductive Nano-hybrid structures and its composite for flexible electronics

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Abstract

Recent advancements in flexible electronics have emphasized the importance of materials that combine mechanical flexibility with high electrical conductivity. Conductive nano-hybrid structures, consisting of nanoscale building blocks such as carbon nanotubes (CNTs), graphene, metal nanoparticles, and conductive polymers, offer unique advantages for this purpose. These materials can be engineered to exhibit remarkable electrical, thermal, and mechanical properties, making them ideal candidates for next-generation electronic devices.
The present study aims at the synthesis of various nano-hybrid structures with polymer-based composites, which are commonly used for their flexibility and durability. Combining these nanostructures enhances electrical conductivity, mechanical resilience, and stability under deformation. Furthermore, the synergistic effect between the nanomaterials and the matrix polymers allows for improved performance in wearable devices, sensors, and energy storage systems.

A1-0115

Surface Plasmon Induced Enhanced Optical Limiting Activity in One-Dimensional Au-PTCDI-C8 Nano-systems

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Abstract

The incorporation of plasmonic nanoparticles into π-conjugated organic semiconducting materials to modify their intrinsic optical responses has garnered significant attention in research. Here we report, the enhanced optical limiting response of N,N′-Dioctyl-3,4,9,10-perylenedicarboximide (PTCDI-C8) nanoribbons integrated with Au nanoparticles (NPs). Optical limiting response was monitored by open-aperture Z-scan technique using a Q-switched Nd laser with a wavelength of 532 nm and a pulse width of 7 ns. The optical limiting threshold (the input fluence at which output transmittance become half of the initial) of Au-PTCDI-C8 nanohybrid is found to be 1.75 J/cm2 which is higher that its constituents. The improved nonlinear optical activity was ascribed to the strong reverse saturable absorption (RSA), that was the outcome of a synergistic interaction between the characteristic excitonic transition of PTCDI-C8 nanoribbons (506-536 nm) and the intrinsic plasmonic oscillations of Au nanoparticles (470-580 nm). On integrated Au- PTCDI-C8 nanoribbons, an enhancement of ~ 60 times in the electric field intensity near Au nanoparticles was observed theoretically using FDTD analysis, which is also believed to be responsible for their enhanced optical limiting responses of the nanohybrids. The optical limiting threshold of Au- PTCDI-C8 on par with or better than recently reported π-conjugated and nanohybrid materials, demonstrating the effectiveness of this approach in developing novel optical nanomaterials with outstanding nonlinear absorption properties.

A1-0116

Growth and Characterization of V_2O_5 Nanoflowers on cobalt Coated Silicon Substrate

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Abstract

This report explains the growth of vanadium pentoxide (α-V_2O_5) nanoflowers (NFs) on pre-deposited MoO_3 nanoplates (NPs) using Plasma Assisted Sublimation Process (PASP). The growth process occurs into two consecutive growth steps on cobalt (Co) coated Si substrate. In first step, vertically aligned nanoplates (NPs) of MoO_3 are deposited uniformly on entire substrate. The second step involves the growth of vanadium oxide NFs on already grown MoO_3 NPs using the same PASP. The recorded set of peaks in X-ray diffractogram (XRD) of film after step II, divulges that only orthorhombic phase of vanadium oxide (i.e. α-V_2O_5) is present. The high intensity along with sharp full width and half maxima (FWHM) of peaks, ascertain the excellent crystallinity of film and also ensures that preferred direction of crystal growth is long b-axis. SEM images of films in both the steps are recorded separately. After first step, the image shows the growth of vertically aligned MoO_3 NPs with excellent aspect ratio (~ 30) whereas; the uniform growth of α-V_2O_5 NFs over MoO_3 NPs is occurred in second step. The Raman and FTIR spectra of NFs show various absorption bands and all are assigned according to orthorhombic phase of vanadium oxide. The remarkable red shift in Raman peaks confirms the existence of low oxidation state of vanadium (i.e. V^{4+} & V^{3+}). HRTEM and SAED show the single crystalline nature of NFs with 0.34 nm interplanar spacing and again infers that α-V_2O_5 NFs grows preferentially along [010] direction. Growth mechanism of NFs is also discussed in brief.

A1- 0117

Optimizing Solar Cell Efficiency via Downconversion: Current Trends and Future Directions

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Abstract

The optimization of solar cell efficiency is a vital area of research as the demand for renewable energy surges. This review focuses on downconversion techniques, which convert high-energy photons from the solar spectrum into lower-energy photons that can be more effectively harnessed by photovoltaic cells. We analyze current trends in downconversion materials, including organic phosphors, inorganic nanocrystals, and quantum dots, highlighting their potential to enhance light absorption and minimize thermal losses. Key strategies for integrating these materials into various solar cell architectures are discussed, showcasing notable improvements in power conversion efficiency in recent studies. Additionally, we address the challenges associated with material stability, integration, and manufacturing scalability, while identifying promising avenues for future research, such as novel nanostructured materials and advanced design methodologies. By synthesizing recent advancements and proposing future directions, this review aims to illuminate the transformative potential of downconversion technologies in the ongoing pursuit of highly efficient solar energy solutions.

A1- 0118

Advancements in Sol-Gel Synthesized BiFeO3 Nan particles: Impact on Multiferroic Properties over the Past Decade

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Abstract

Over the past decade, multiferroic BiFeO3 (BFO) nanoparticles have emerged as a critical material for studying coupled ferroic orders due to their unique coexistence of ferroelectricity and antiferromagnetism at room temperature. This review examines the advancements in the synthesis of BFO nanoparticles using the sol-gel method, focusing on how variations in synthesis parameters-such as precursor concentration, annealing temperature, and dopants-affect their multiferroic properties. The sol-gel technique offers advantages in controlling particle size and morphology, both of which significantly influence the electrical, magnetic, and magnetoelectric coupling properties of BFO. A key observation is that reducing particle size to the nanometer scale results in enhanced ferroelectricity and weakens magnetic leakage, attributed to surface effects and size confinement. Additionally, the incorporation dopants like rare earth elements has been shown to stabilize the perovskite phase and mitigate the leakage current problem, leading to improved multiferroic performance. This review synthesizes findings from the last ten years, highlighting the challenges and opportunities for optimizing BFO nanoparticles for applications in spintronics, memory devices, and sensors. The analysis underscores the importance of fine-tuning the sol-gel synthesis process to achieve the desired phase purity, dielectric properties, and magnetoelectric coupling essential for advancing the practical utility of BFO-based materials.

A1- 0119

A Review on the Green Synthesis of Metal Oxide Nanoparticles for Antimicrobial Activity Using Different Plant Parts

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Abstract

In recent years, green chemistry has witnessed a surge towards sustainable approaches for nanoparticle synthesis. Researchers are now exploring the potential of diverse plant extracts to produce ecological nanoparticles. Biomedical sciences are paying more attention to synthesizing different metal oxide nanoparticles mediated by plants and their wide biological uses. Plant-mediated biogenic synthesis of metal oxide nanoparticles is an ecologic, less harmful and low-cost method; additionally, it has advantages for biological analysis regarding antifungal and antibacterial activities. Plants contain diverse phytochemicals, including amino acids, polyphenols, flavonoids, and terpenoids which can act as both reducing and stabilizing agents. However, the mechanism of green synthesis using plants is still extensively discussed. In this report, several nanoparticles like zinc oxide (ZnO), titanium dioxide (TiO_2), iron oxide (FeO), nickel oxide (NiO), and copper oxide (CuO) offer essential insights into their antimicrobial activity against various bacterial strains in different concentrations. Additionally, the research delves into uncovering the mechanism that promotes antimicrobial effects.

A1- 0120

Promises, Problems, and Path-ahead for Ga_2O_3 and –based Electronics

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Abstract

With the ever-increasing expansion of power electronics in our day-to-day applications, it demands more efficient power electronics. Ultra-wide bandgap semiconductors such as gallium oxide (Ga_2O_3) can provide energy-efficient power electronics. Relatively easier/cheaper single crystal growth and epitaxial growth method for Ga_2O_3. The β-phase is the most stable of its five phases (some say six) and it has very attractive properties. It has many advantages over conventional semiconductors like Si, GaN and SiC. At the same time, there are a few challenges which need to be overcome for Ga_2O_3 to become the leading semiconductor for power electronics. Other than power electronics, Ga_2O_3 semiconductor has been used for different niche application areas. We will discuss the different prospects, scope, and future direction of Ga_2O_3. For example, very few works have reported two-dimensional electron gas (2DEG) in this system. Success of AlGaN/GaN technology lies in the excellent property of the 2DEG formed at the heterointerface. Investigating the feasibility of 2DEG formation and optimization of 2DEG at interface of Ga_2O_3 will pave the way for implementation of Ga_2O_3 HEMT and utilizing its true potential for electronic applications. We will discuss different possible approaches to achieve 2DEG in Ga_2O_3.

A1- 0121

Influence of Nanopartcles and Their Role in Enhanced Oil Recovery

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Abstract

With the advent of nanotechnology, nano - metric sized particles and their use is not limited to food and agriculture sector but nowadays they found application in diverse sectors such as crude oil industry and in advanced methodologies of oil recovery. This paper presents the impact of different nanoparticles being in use by petroleum industry to increase the oil recovery and also enhance the various oil characteristics such as viscosity, API, etc. The work elaborately describes the detailed analysis of the use of nanoparticles in improving the various drilling fluid properties like rheological characteristics, foam stability and improving the lubrication of the well drilling fluids. Promising results were observed due to the distinctive characteristics of nanoparticles such as increased surface area to volume ratio. Despite, promising results, still the mechanism of enhanced oil recovery is a mystery for the researcher which needs to be explored. The application of nanotechnology needs to be focused and employed in various sectors of petroleum industry such as exploration, drilling, reservoir, completion, production, and oil recovery in each stage. This paper emphasizes on giving a concise thought over the significant uses of nanoparticles, their potential advantages, associated economic and technical challenges, and solutions.

Keywords: Nanoparticles, oil recovery, API, viscosity, crude, rheological, stability

A1- 0122

The structural, electrical properties, conductive grains and NTCR behaviour via impedance spectroscopy in of 1-x ($Na_{0.5}Bi_{0.5}TiO_3$)-x ($BaTiO_3$) solid solution

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Abstract

1-x ($Na_{0.5}Bi_{0.5}TiO_3$)-x ($BaTiO_3$) ceramics were prepared by using a solid-state reaction method at 950°C for 2hr. Dielectric permittivity (ε′) was observed with frequency at different temperatures, with a decrease in ε″ due to the decrease of net polarization. The Havriliak-Negami model fits both real and imaginary parts of dielectric permittivity at all temperatures (RT-500°C) due to reduced space charge polarization effect at grain boundaries. A peak in the temperature range between 100 to 200°C was observed, possibly due to space charge polarization. The higher ionic radius of the Ba^{2+} ion compared to the $(Na_{0.5}Bi_{0.5})^{2+}$ ion introduced local strain, supporting the formation of polar regions responsible for relaxor behavior. Complex impedance analysis suggested the presence of NTCR (negative coefficient of resistance) in the sample in the low-frequency region, merging at almost all temperatures in the high-frequency region. The imaginary part of impedance changes with frequency at different temperatures, indicating temperature-dependent dielectric relaxation. The focus will have been on understanding how the variation in composition influences the sample's conductive grains, grain boundaries, and NTCR behavior, providing a comprehensive understanding of the electrical and thermal properties that make this system suitable for advanced technological applications.

Keywords: Ferroelectric, NTCR, Dielectrics, Structural Studies, Perovskite, Complex impedance.

A1-0123

Structural and optical properties of Mn-doped Cu ferrite nanoparticles.

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Abstract

The Mn-doped copper ferrite nanoparticles, a novelmaterial of significant interest in green chemistry, standout for their exceptional properties, including their biocompatibility, and minimal environmental impact. This study is crucial for understanding their potential applications, focuses on the structural and optical properties of these nanoparticles (MCFNPS). The research conducted using X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR), confirms the unique features of these nanoparticles. The conventional auto-combustion method was used to synthesize MCFNPS, and the results shows that the nanoparticles exhibit a cubic spinel structure, with particle sizes ranging from 50 to 60 nanometers, and no secondary phase was observed. The FTIR studies revealed octahedral and tetrahedral bond vibrations, providing evidence of spinel structure formation. In conclusion, the synthesized MCFNPS possess a single-phase spinel cubic structure, making them potentially suitable for medical applications.

Keywords: Magnetic materials, Ferrites, XRD, FTIR

A1-0124

Solitons in Discrete Waveguides

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Abstract

We analyse soliton stability in discrete waveguides, revealing the impact of waveguide parameters and nonlinearity. Our analysis reveals the impact of waveguide parameters and nonlinearity on soliton stability, identifying design guidelines for stable propagation.

Key words: soliton stability, discrete waveguides, nonlinearity, design guidelines.

A1- 0125

Exploring the Structural, Electrical, and Optical properties of Rare-Earth Orthochromites ($RCrO_3$, R=Nd, La) prepared by chemical route

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Abstract

In the present work, we have synthesized perovskite-type samples $NdCrO_3$ and $LaCrO_3$ by using chemical combination method. The prepared samples were characterized by TGA and were annealed at 750^0c for 1 hour in a muffle furnace. Then the structural and microstructural characterizations were done by X-ray diffraction (XRD), Scanning Electron Microscopy (SEM) and Energy Dispersive Spectroscopy (EDS), respectively. From XRD analysis, it is observed that the X-Ray diffraction of $NdCrO_3$ and $LaCrO_3$ powder peaks match with ICDD Card No.-01-088-0695 and 01-083-1327 having an orthorhombic crystal system with pnma space group (no. 62) respectively. By the Scherrer equation the average crystallite size of $NdCrO_3$ and $LaCrO_3$ is about 17.39nm and 22.13nm. From SEM analysis dense microstructure with grain boundaries is observed. Grains are having non-uniform distributions. Energy-dispersive X-ray spectroscopy of the $NdCrO_3$ sample shows the presence of Nd, Cr and O elements. The electrical impedance and dielectric properties of the materials were investigated in the range of temperature (30^0C-400^0C) and frequency of (50 Hz-8 MHz) using LCR Meter. This rare-earth orthochromites represent a fascinating class of materials with diverse properties. Due to their unique fundamental properties like ferroelectric, piezoelectric, colossal magnetoresistance, multi-ferrocity enhances their performance for modern technology applications.

Keywords: Orthochromites, chemical combination method, XRD analysis and impedance measurement

A1- 0126

Theoretical Insights into Stibine Gas Adsorption and Desorption on Stanene Monolayer for Gas Sensing Applications

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Abstract

Using DFT calculations, we have successfully examined the adsorption of stibine gas molecules on a stanene 2D sheet. Detecting stibine is crucial due to its toxic and hazardous nature, making efficient sensing technology vital for environmental safety. The adsorption energy was found to be -0.62 eV, indicating a stable interaction. The charge transfer from the molecule to the sheet was 0.04 e, suggesting a slight electron transfer upon adsorption. Additionally, the recovery time for desorption is 3.058×10^{-2} s, demonstrating the dynamic response of the material. These findings highlight that the stanene 2D sheet is dynamically stable and effective as a gas sensor. The strong chemical interaction is further supported by the overlap in the density of states between the interacting atoms. Our results provide valuable insights for developing promising gas sensor devices based on the stanene 2D sheet.

A1- 0127

Development of Nano-Robots Utilizing Nano Materials and Smart Materials for Targeted Cancer Treatment in Medical Applications

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Abstract

The main objective of the nanorobotic project is to design a miniaturized Magnetic Nano-Robot (MNR) for detecting cancerous cells using simulation tools such as Nano-Hive, incorporating biomolecules like carbon nanotubes (CNTs), lipids, pH/O2/Ferro Magnetic Nano Particles encapsulated in silk proteins. The MNR aims to detect affected cells via bio-sensors, release targeted cancer drugs to the tumor, and disinfect the area. The project involves testing the fabricated MNR prototype across various stages, including laboratory, animal, and human trials at institutions like IISc, NCBS, and SCH. Following successful trials, the goal is to apply for a patent, publish findings, secure grants, develop a start-up, and eventually release the product to the market. To achieve these goals, the research follows ten critical measures: determining the nanorobot's mode of entry into the human body; developing a propulsion system for the nanorobot; ensuring the ability to hold a set location while working; determining the operational use of the system; finding a suitable power source for the nanorobot; accurately locating the infected cell in two scenarios (moving with and against the fluid flow); identifying methods for removing compounds targeted by the nanorobot; establishing procedures for drug removal from the body; continually observing the body and updating on the cancer cell's destruction; and ultimately rendering the infected cell inactive or extracting it from the human body. Problem statement of the project is to design a miniaturized MNR to detect the cancerous cell using simulation tools like nano-hive with the help of biomolecules (CNTs, lipids, pH/O2/Ferro Magnetic Nano Particles encapsulated silk proteins) and detect the affected cell using bio-sensors, release the cancer drug to the tumour and disinfect it along with the testing of fabricated MNR prototype model (lab, animal, human) in the IISc lab/NCBS/SCH. The body obtains its own strength in a similar manner by absorbing fuel chemicals from the bloodstream. The figure shown encompasses the fabrication process of nanorobots and utilizes AI and ML approaches for training purposes and the development of the project's flow chart, detailing the methodology and concepts used for the virus’s destruction.

A1- 0128

Chemical Decomposition Method of Designing and Development of a Nano Antenna for Energy Harvesting in Internet of Things Dependent Nanotechnology Systems using nanopowders

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Abstract

This research article presents the development of nano antennas for energy harvesting. With the increasing prevalence of wirelessly interconnected devices, the Internet of Things (IoT) is becoming a significant part of modern society. These devices, which often operate autonomously, are continually scaling down to millimeter and even smaller dimensions, creating substantial challenges for powering them. To address this, various energy harvesting approaches have been developed, including radio-frequency, optical, mechanical, thermal, nuclear, chemical, and biological modalities. This article provides a comprehensive survey of these methods, discussing their potential to scale down to small dimensions within the context of current technologies and future nanoscience advancements. As the number of untethered, wirelessly interconnected devices grows, the IoT has seen widespread adoption. These autonomous devices, which range from millimeter to sub-millimeter sizes, present significant power supply challenges. In this article, we conduct a thorough survey of current energy harvesting methods, covering modalities such as radio-frequency, optical, mechanical, thermal, nuclear, chemical, and biological sources. These methods enable the generation of electrical power for micro- and nano-systems. We explore the potential for scaling these energy conversion techniques to smaller dimensions, taking into account existing technologies and future developments in nanoscience. Additionally, the article provides an outlook on necessary advancements to overcome the challenges of powering small-scale devices and systems.

Keywords - Photovoltaic devices, Infrared, Communications, Nano antennas, Lithography, Chemical, etc.

A1- 0129

A Silkworm Counting Method with Density Map Based on Multiscale Feature Fusion in Small Worms Using Physics based Nano-Materials

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Abstract

Silkworm rearing is integral to our agricultural heritage and deeply rooted in Han culture. Accurate counting of silkworms is crucial for optimizing silk production. Traditional counting methods, relying on visual inspection and experiential estimation, are prone to inaccuracies and resource inefficiencies. In response, this study introduces the Silkworm Counting Network, a novel approach aimed at generating density maps and precisely tallying silkworm populations. Using images from the sericulture area of Guangxi, a diverse silkworm dataset was meticulously curated, covering various age groups and backgrounds. Data augmentation techniques were applied to enhance dataset diversity, ensuring robust model performance. The front-end network employs the VGG architecture for feature extraction and integrates multi-scale contextual semantic information extraction modules to enrich silkworm features. The back-end network utilizes dilated convolutions with varying rates to expand the receptive field and generate silkworm density images for accurate counting. Evaluation of the proposed method on the constructed silkworm density dataset demonstrates promising results, with a root mean square error (RMSE) of 8.5 and mean absolute error (MAE) of 5.3. By overcoming challenges such as occlusion and varying population distributions, the proposed approach transcends conventional target detection methods. Density map-based counting proves superior in estimating silkworm density per unit area, enabling more accurate quantification than simplistic number statistics. A review of related works highlights the scarcity of research in silkworm density statistics, primarily focusing on dense crowd and object detection.

A1- 0130

The persuasive consequences of Optical, Dielectric and Photoluminescent properties of Cholesteric Liquid Crystal by the dispersion of Zinc Oxide (ZnO) nanoparticles

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Abstract

A multifaceted system of Zinc oxide (ZnO) nanoparticle dispersed cholesteric liquid crystals revealed the augmented investigations. The significance of dispersion of ZnO nanoparticles at different concentration is very extensive in the cholesteric liquid crystal. Thermodynamical investigation revealed the reduction of transition temperature and enthalpies of different liquid crystal phases. Electro-Optical behaviour of ZnO doped cholesteric liquid crystals shows the arrangement of molecules by applying the electric field. Dielectric investigation documented outcomes of ZnO nano particles doped cholesteric liquid crystal at the biasing. Dielectric studies exhibit the signature of the soft mode (SM) and relaxation process of molecules in liquid crystal phases. ZnO nanoparticles doped cholesteric liquid crystal enhanced the efficiency area of doped complex material surface. The increment of Intensity of photoluminescence is responsible due to the functionality of nano particles in cholesteric liquid crystals system.

Key Words: ZnO Nanoparticles, Soft Mode, Relaxation process Photoluminescence,

A1- 0131

Synthesis of Nickel Selenide Nanoparticles as Cathode Material for Zinc Ion Batteries and Study of Their Optical Properties

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Abstract

Porosity of electrode materials has been proven to be very significant in enhancing the performance of Zn-ion batteries (ZIB) in recent studies. On a positive electrode, porosity improves its kinetics by faster electron transport and richer electro active reaction sites. On a negative electrode, porous structure provides increased surface area and reduced local current density, both favorable to the performance of ZIB. Nickel Selenide (NiSe) nanoparticles can be considered as more suitable cathode materials also due to their smaller band gap and higher conductivity. We have synthesized NiSe nanoparticles using a chemical method with octylamine as a surfactant with crystallite size of 36 nm. The field emission scanning electron microscopy (FESEM) images shows the formation of spikelike structure making the nanoparticles highly porous making them even more suitable as a cathode material.

A1- 0132

A Study of Green Mediated Synthesis of Cu-doped ZnO Nanoparticles: Structural and Optical Properties

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Abstract

Nanocrystalline Cu-doped ZnO particles were synthesized using green synthesis technique using Jatropha Plant latex. The effect of precipitating agent's sodium hydroxide (NaOH) and ammonium hydroxide (NH_4OH) on the structural and optical properties has been studied. The composition, structural and optical characterizations were examined by X-Ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and UV-Visible spectrometer. From the XRD results it is confirmed that nanocrystalline Cu-doped ZnO particles have a hexagonal wurtzite structure with a high crystallinity. The FT-IR analysis confirmed the presence of functional groups such as -OH stretching vibration of phenol and hydroxyl group, CH stretching, C=C stretching of alkyl ether group, C-N stretching of aromatic amine in the plant extract. The UV-visible confirmed that ZnO nanoparticles have a direct energy band gap which decreases with increasing the Cu concentration from 2.5 wt% and 10wt%. The result confirms that the doping of Cu in pure ZnO nanoparticles (NPs) changes their average crystal size (13-14 nm) with NaOH and NH_4OH is 27-34 nm. The shift in the excitation and emission spectra towards the visible region of the electromagnetic spectrum was observed in the presence of both precipitating agents, as compared to pure ZnO. This study highlights the effect of precipitating agents on the modification of different properties of plant mediated synthesized nanomaterials.

A1- 0133

Study of the temperature dependence of transport characteristics in LCMO (perovskite manganite) - rGO nanocomposite system

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Abstract

Intensive studies of resistive switching mechanisms in oxide systems have gained extensive research interest due to its great potential prospect in non-volatile memory applications. There are many materials which are well-explored for the RS phenomenon as binary oxides, polymers, perovskites, chalcogenides and even 2-D materials. The investigation for the best material offering RS behavior is steel going on some magnetite like (Pa0.7Ca0.3Mn03La0.7 Sr0.3Mno3) also depicts the RS behavior and their performance are limited by the random. Oxygen vacancies perform a vital role in initiating the resistive switching (RS) phenomenon in oxide-based systems. The random oxygen vacancies can be limited by two methods (1) by dopping and (2) by forming nanocomposite. Interest has grown in understanding to perovskite material. Among the several oxide materials, oxygen vacancies are introduced in oxide-based systems using the synthesis method itself. So lanthanum calcium manganites (La0.3Ca0.7MnO3) are taken as active materials due to their fascinating physical and electrical properties and study its RS effects, the small amount of reduced graphene oxide (rGO) in it.

A1-0134

Magnesium Adsorption on B/N/P-Doped Graphene Nanoribbons: A DFT Investigation of Structural and Electronic Modifications

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Abstract

The interactions of magnesium (Mg) atoms adsorbed on boron (B), nitrogen (N), and phosphorus (P)-doped zigzag (ZGNR) and armchair graphene nanoribbons (AGNR) are investigated using density functional theory (DFT). The study examines the adsorption characteristics of Mg on doped GNR surfaces, revealing physisorption due to weak vander walls forces, in contrast to the chemisorption observed for lithium on B/N/P-doped AGNRs. The adsorption energies for Mg on B, N, and P-doped AGNRs are calculated as -3.37 eV, -2.86 eV, and -0.21 eV, respectively, with B-doped AGNR showing the strongest interaction. The adsorption energy for lithium on B-doped AGNR (-3.72 eV) is similar to that of Mg. Further, the Mg-B interaction results in a shorter bond length compared to Mg-N resulting in better adsorption behavior. However, in the case of P doping, the heavier atomic weight of P leads to surface deformation. Additionally, Mg adsorption significantly reduces the bandgap of all doped AGNRs, transforming them into metallic conductors with enhanced conductivity. This study suggests that Mg-doped GNR systems could offer a viable alternative for applications traditionally reliant on lithium.

Keywords: Doped graphene nanoribbon, Magnesium adsorption, Adsorption energy, DFT

A1-0135

Synthesis, Characterization and Applications of ZnO as a piezoelectric material

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Abstract

In this research, ZnO nanoparticles were created through hydrothermal and sol-gel methods.Both approaches provide distinct reaction conditions, resulting in differences in the structural and morphological characteristics of the ZnO particles.
The hydrothermal approach required zinc precursors to react in high-temperature, high-pressure settings, whereas the sol-gel method utilized a chemical pathway where a zinc precursor underwent hydrolysis and condensation to create a gel, which was then subjected to calcinations to produce ZnO nanoparticles.
The synthesized ZnO particles were analyzed with X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). XRD analysis validated the crystalline structure and phase purity of the ZnO nanoparticles, while SEM gave information on the surface morphology, showing particle size distribution and shape. TEM was used for a thorough analysis of the inner makeup and nano-level characteristics, such as particle dimensions and structure of being crystalline. The contrast between the two procedures reveals variations in particle dimensions, structure, and crystal form, underscoring how the synthesis parameters impact the characteristics of ZnO. This study seeks to take advantage of the intriguing characteristics of ZnO on a nanoscale, as a wide-bandgap semiconductor. It aims to utilize ZnO as piezoelectric materials to convert mechanical energy into electrical energy and gather this generated electricity.

A1- 0136

Optimizing Annealing Temperature for Tailored Structural and Optical Properties of 2D $ZnGa_2O_4$ Nanosheets Synthesized via Hydrothermal Method

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Abstract

$ZnGa_2O_4$ nanosheets were successfully synthesized using a simple hydrothermal method, generating interest in their 2D nanostructures due to their promising physical and chemical properties for a wide range of applications. Investigation into the impact of annealing temperature on structure, morphology, and optical activity revealed distinct findings. The XRD spectrum exhibited diffraction peaks characteristic of fcc-type $ZnGa_2O_4$, while EDS spectra highlighted Zn, Ga, and O elements. Samples annealed at 750 °C and 800 °C displayed additional peaks near 2θ positions of 31.5° – 32.5°, 34° – 34.5°, and 36.1°-36.8°, suggesting inadequate annealing for Zn^{2+} inclusion in the Ga_2O_3 structure, given their disparate atomic radii (0.74 Å and 0.63 Å). At 850 °C, the absence of impurities confirmed the phase purity of the synthesized $ZnGa_2O_4$ nanosheets. SEM images depicted triangular/hexagonal structures with ultrathin thickness, exhibiting preferential growth in the (111) plane due to minimum formation energy. TEM analysis reveals well-crystallized nanosheets with fcc-type spinel structure symmetry. FTIR spectra supported metal oxide bonding and functional group prevalence. This study highlights the hydrothermal method's simplicity and precise control in fabricating 2D semiconductor nanosheets, offering significant potential for advancing optoelectronic applications through optimized annealing conditions.

A1- 0137

Eggie Sense - Smart Egg Health and Quality Monitoring System Development for Health Applications using Bio-Materials

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Abstract

This paper presents EggSense, an IoT-based system for real-time monitoring of egg quality and health. Using an Arduino/ESP32 platform and Blynk, EggSense integrates infrared (IR) LEDs to measure egg protein content and a camera module for image processing to detect diseases by identifying shell abnormalities. The system provides real-time data visualization and alerts via a mobile interface, enabling remote monitoring. EggSense offers a non-invasive, efficient solution for improving egg quality control in the poultry industry. This paper discusses the design, implementation, and potential benefits of the systems. This paper introduces EggSense, an innovative IoT-based system designed for the real-time monitoring of egg quality and health in the poultry industry. The system is built on an Arduino/ESP32 platform, utilizing Blynk for mobile connectivity, and integrates several advanced components to ensure comprehensive monitoring. EggSense employs infrared (IR) LEDs to assess the protein content within eggs, providing crucial insights into their nutritional value. In addition, the system is equipped with a camera module capable of performing image processing to detect diseases or irregularities by identifying abnormalities in the eggshells. This combination of sensor-based data collection and image analysis ensures that egg quality is monitored non-invasively, with real-time updates accessible via a mobile interface. The system offers several advantages, particularly in its ability to provide real-time data visualization and immediate alerts, allowing for remote monitoring and swift intervention when issues arise. This capability enhances the efficiency and accuracy of quality control processes in the poultry sector, reducing reliance on manual inspection and enabling producers to address problems early. The paper explores the complete design and implementation of the EggSense system, discussing its hardware and software components, data processing techniques, and integration with mobile platforms. Furthermore, it highlights the potential benefits of adopting EggSense, such as improved egg quality, better disease management, and increased operational efficiency, making it a valuable tool for modern poultry farms.

A1- 0138

Synthesis and Characterization of CuO: SnO2 Composite nanoparticles for Photocatalysis Activity to Degradation of Methylene Blue Dye

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Abstract

The novel CuO-SnO2 nanocomposite oxide photocatalysts were prepared by simple co-precipitation method, and characterized by X-ray diffraction, Scanning electron microscopy, FTIR and UV-visible spectroscopy. The photocatalytic activities of CuO-SnO_2 evaluated using the photodegradation of Methylene Blue under UV- visible lam. The photocatalytic activity of the synthesized CuO-SnO_2 photocatalyst was observed at different calcinated temperature (300°C , 400°C , 500°C)for 3h, with the molar ratio of Cu to Sn is 1:1 .It shows that degradation of methylene Blue dye is higher for composite sample crystalline at higher temperature. It also showed much higher photocatalytic activity in treatment dye wastewater under normal sunlight irradiation.

Key Word: Copper Oxide, Tin Oxide, Nano particles, Characterization, photocatalysis

A1-0139

Fractal, Optical, and phonon modes of Ti2C films deposited by dc-magnetron sputtering

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Abstract

Titanium dicarbide (Ti2C) thin films (~150 nm total thickness) were deposited using a dc-magnetron sputtering system. The RMS roughness of the tetra layer films was 4.1 nm. The fractal varied from 1.931 to 2.519 of Ti2C thin film. Raman analysis showed the TA, LA, and TO Raman bands at 234, 333, and 629 cm-1, respectively. The D-band and G-band were observed at 1326.87 and 1587.14 cm-1 respectively. The UV-vis spectra indicate the Tauc band gap of 3.43 eV and Cody band gap of 3.49 eV of Ti2C thin films. X-ray absorption spectroscopy confirmed the Ti L- edge, C-K-edge, and O K- edge was observed at 462.30, 287.31, and 538.13 eV in the Ti2C thin films.

Keywords: Ti2C Films, Sputtering, Fractal analysis, Optical properties, Phonon Modes

A1-0140

Transport Properties of n-Type Thallium-Doped Bi_2Se_3 Nanoparticles

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Abstract

Bismuth Selenide (Bi_2Se_3) has wide range of applications in thermoelectric and optoelectronic devices. This study is focused on synthesis and characterization of Thallium doped Bi_2Se_3 nanoparticles synthesized via the hydrothermal method. The structural properties were examined using X-ray diffraction (XRD) and Fourier-transform infrared (FTIR) spectroscopy. The optical properties were obtained using Diffuse reflectance spectroscopy (DRS). Additionally, the transport properties were measured using Hall Effect at room temperature and thermoelectric power measurements between room temperature to 160 $^{\circ}$C. The developed material is currently being explored for device fabrication for thermoelectric sensors.

A1-0141

Comparative Analysis of Water-Based ZnO and Ag Nanofluid Flow Over a Steady Stretching Cylinder with Slip and Suction Effects

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Abstract

The paper presents a comparative analysis of the laminar, two-dimensional flow of water-based ZnO and Ag nanofluids over a stretching cylinder. Key effects such as magnetic field, porous medium, mixed convection, viscous dissipation, Joule heating, and thermal radiation are considered. Velocity slip and suction/blowing at the surface are also included. The governing equations are reduced using similarity transformations and solved numerically via the bvp4c method. The study explores how nanoparticle volumetric fraction (ϕ) affects velocity, temperature, skin friction, and the Nusselt number, providing insights through graphical and tabular analysis. These findings are applicable in optimizing heat transfer systems for industrial processes involving nanofluids.

Keywords: Nanofluid, Magnetic field, Thermal radiation, Velocity slip, Joule heating, Heat source/sink, Porous medium, skin friction, Nusselt number.

A1-0142

Structural, Electronic and Elastic Properties of α-Mg_3N_2: A First Principle Study

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Abstract

In this study, the Linear Combination of Atomic Orbitals (LCAO) method is applied to explore the structural, elastic and electronic properties of the α-Mg_3N_2 compound. Using the Density Functional Theory (DFT) within the Generalized Gradient Approximation (GGA) framework, structural parameters are optimized to determine its structural characteristics. This investigation reveals that α-Mg_3N_2 exhibits semiconducting behavior based on its electronic properties. With an energy band gap that falls within the optimal range for the solar spectrum, α-Mg_3N_2 emerges as a promising material for photovoltaic applications.

Key Words: Semiconductor, Electronic structure, LCAO method, Band structure, Elastic

A1-0143

A Review paper on Friction Stir Processing (FSP) of Al 5083 Aluminium alloy

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Abstract

The process of Friction Stir Processing (FSP), which was originated from Friction Stir Welding (FSW), is used to improve the mechanical and microstructure characteristics of materials. It creates dynamic recrystallization and localized plastic deformation by introducing a rotating tool with a pin and shoulder into the material. Grain structure is improved through this technique, leading to increased ductility, formability, and mechanical strength. FSP has gained prominence for its ability to modify microstructures without the need for fusion or heat treatment, making it ideal for processing metals like aluminum alloys.

In this review, the focus is on the application of FSP on Al 5083 alloy, widely used in industries such as marine, aerospace, and transportation due to its excellent corrosion resistance and mechanical properties. The article describes several methods for creating surface and hybrid composites utilizing Friction Stir Processing (FSP). Surface composites are highlighted because they have improved surface characteristics, such as fatigue life and abrasion resistance, while retaining the bulk properties of the base material.

The advantages and disadvantages of certain fabrication methods such as the groove and hole approaches are discussed in order to achieve a consistent distribution of reinforcement. The impact of process parameters on the microstructure and grain refinement, such as tool rotation and pass speed, are also covered in this paper. All things considered, FSP is offered as a flexible and sustainable practices way to modify the microstructure of materials to create high-performance materials.

Keywords: - Friction Stir Processing (FSP), Al 5083 Alloy, Surface Composite, Hybrid Composite, Process parameters.

A2-0001

Metric f(R) Gravity and Black Hole Evolution: A Theoretical Exploration

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Abstract

In this work, we have employed Power-law cosmology to investigate both the accelerated expansion of the universe and black hole dynamics within the framework of Starobinsky-type metric f(R) gravity. Specifically, we have examined the variation of black holes size due to accumulation of energy-matter from the surroundings, named as accretion of black holes, during different cosmic eras. Our finding suggested that a higher accretion rate leads to greater mass loss of black holes. Notably, our analysis reveals that certain black holes could completely evaporate at a particular time, regardless of their initial formation mass.

A2-0002

Critical Mass Thresholds for Neutron Star Stability and Black Hole Formation in Gravitational Collapse

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Abstract

This research investigates the critical mass thresholds for black hole formation during the gravitational collapse of massive stars. Employing numerical simulations and analytical techniques, we find the conditions under which gravitational collapse leads to black hole formation. Utilizing the Tolman-Oppenheimer-Volkoff (TOV) equation, we model the collapse of a spherically symmetric, non-rotating neutron star with a customized density profile predicted in our previous paper. In this paper, we have also performed analytical solution of TOV equation considering density to be constant. When applying the TOV equation with a constant density of 1.6×1018 Kg/m3, the maximum mass of neutron star is estimated to be 2.85 solar masses. Incorporating the customized density profile into the TOV equation, the result comes out as critical mass of neutron star to be 2.096 solar masses at a radius of approximately 10 km, consistent with current theoretical and observational expectations. The maximum mass is calculated as 2.36 solar masses, with the mass dropping to zero beyond a radius of 15.5 km. By comparing different initial masses (2.0, 4.0, and 8.0 solar masses) and employing polytrope EOS, we analyze the mass-radius and pressure-radius variations, explaining the influence of mass on stellar stability. This reveals that the structure of a relativistic star can exhibit a highly non-linear and abrupt change in both mass and pressure distributions. The significant increase in mass and pressure at specific radial distances suggests the presence of a dense outer shell. This research provides valuable insights into neutron star stability limits and the conditions for black hole formation.

A2-0003

Co-Seismic Ionospheric effects of Mw 7.5, Noto Peninsula, Japan Earthquake, of 01 January 2024

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Abstract

This study investigates the co-seismic ionospheric variations observed during the Japan earthquake of Mw7.5 that occurred on 01 January 2024 at 07:10:55 (UTC). For this purpose, the total electron content (TEC) data are computed from three IGS stations, i.e. DAEJ in Korea, MTKA, and USUD in Japan. The TEC variations revealed significant anomalies corresponding to this earthquake. The DAEJ station is 887.4 km from the epicenter, MTKA is 286.7 km, and USUD is the closest station, i.e. 179.15 km from the epicenter. The anomaly was first observed at the USUD station with a change in TEC of about 0.12 TECU after almost 9 minutes of the main event. MTKA Station observed the anomaly after 12 minutes of the main event, with a change in TEC of about 0.065 TECU, and no significant increase in the TEC was observed at station DAEJ. The results are interpreted in terms of the propagation of Acoustic Gravity Waves (AGWs) in the ionosphere during the occurrence of the earthquake. These observations demonstrate the usefulness of TEC monitoring for identifying disturbances in the ionosphere linked to seismic activity. The study reveals that TEC measurements can be a valuable tool in earthquake research, which provides crucial information on the dynamic interactions between seismic events and ionospheric disturbances.

Keywords: AGWs, Total electron content (TEC), Co-seismic ionospheric disturbance (CID), IGS

A2-0004

Ionospheric irregularities corresponding to the geomagnetic storm of 24 April 2023 using global Rate of total electron content (TEC) Index (ROTI) maps

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Abstract

In this paper we briefly summarized the work by different workers on ionospheric irregularities using Rate of Total Electron Content Index (ROTI) and scintillation index (S4). We also studied changes in the global ROTI corresponding to a geomagnetic storm of April 24, 2023. The maximum dip in Dst index was observed at 05:00 UTC with a value of -213 nT. Therefore, the global ROTI maps were analyzed from 23 April to 25 April 2023 at 05:10 UTC. It is to be noted here that the global ROTI maps are available at an interval of 10 minutes. We observed that on April 23, there were severe irregularities in the northern region between 60° and 90°N latitudes while in Antarctica, there were mild irregularities. On April 24, ionospheric activities increased in the northern hemisphere while the southern hemisphere showed moderate disturbances. On April 25, the global ionosphere observed a major decline in disturbances, with calm conditions in the northern polar region and mild disturbances near Antarctica. Throughout the event, the mid-latitude and equatorial regions experience the minimum impact. This study shows an understanding of the temporal evolution of ionospheric disturbances associated with geomagnetic storms, shows variation in how total electron content (TEC) behaves in polar and non-polar regions, and emphasizes the significance of ionospheric disturbances effects on satellite-based navigation and communication systems.

Keywords – ROTI, TEC, Scintillation index (S4), Dst.

A2-0005

Analysis of major geomagnetic storm events and their impact on global total electron content variations during January to June 2023

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Abstract

This study investigates the impact of geomagnetic storms on total electron content (TEC) fluctuations between 01 January 2023 and 30 June 2023. Three significant storms occurred during this period when DST value dropped to -132 nT on 27 February, -163 nT on 24 March, and -213 nT on 24 April 2023. Significant TEC enhancements were found specifically in the equatorial ionization anomaly (EIA) and low-latitude regions by analyzing global TEC (gTEC) maps. During the storm on 27 February 2023, an apparent rise of 20 to 30 TECU was found in TEC values in the Asian region (20^o to 30^o latitudes and -120^o to -90^o longitudes). Similarly, on 24 March 2023 and 24 April 202, the TEC values reached to 40 TECU over the latitudes in EIA region. These results are interpreted in terms of fountain effect at EIA region as during geomagnetic storms, the equatorial electrojet and fountain effect are amplified, resulting in higher electron density and enhanced ionization in certain regions. Additionally, our research points to the possibility of travelling ionospheric disturbances (TIDs), which may be a factor in the localized increases in TEC. This study provides significant new understanding about the behaviour of the ionosphere during geomagnetic disturbances and highlights the significance of observing TEC variations in order to understand the effects of space weather on global communication and navigation systems.

Keywords: TEC, EIA, Ionosphere, EEJ

A2-0006

Response of GNSS Derived Total Electron Content (TEC) During Geomagnetic Storm Of 12 August 2024

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Abstract

This study examines the effects of recent geomagnetic storm of 12 August 2024 (Dst = -203 nT) on total electron content (TEC) over and near geographical equator region. To study this event, the TEC data are computed from three IGS stations at different latitudes namely Diego Garcia Island (UK), Bangalore (India) and Vacoas (Mauritius). The stations considered in this study are representing equatorial and low latitudes. The TEC variations on the event day are compared with averaged TEC values of quietest days of the month. The results show that there is no significant change in TEC at equatorial station, however, changes in TEC increases with increase in latitudes. The percentage change of the difference in event day TEC and averaged quietest days TEC is also calculated and it is found to be varied from 13% to 36%. This change is observed just after the event for both low latitude stations depending on their latitudes but dip is found at the equatorial station. In conclusion, the larger TEC variations were observed at higher latitudes. This suggests the presence of fountain effect in the EIA region. This research work points out the vulnerability of ionospheric TEC arises due to geomagnetic storms and its spatial dependence. This provides insight into the ionospheric character, which could be beneficial for ionospheric corrections required for satellite communication and navigation.

A2-0007

BEC OF NEUTRINO – A DARK MATTER CONSTITUENS

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Abstract

Early prediction of dark matter (DM) by Zwicky in 1930 and then dark energy (DE) are still remaining a mystery. Recently Bose-Einstein Condensate (BEC) which leads to cosmological scalar fields for DE and DM has considered where BEC is collective super atom formed by ultralight bosons. It has been that studied DM as BEC in Minkowski space. A general case was studied rel on curve space time. In BEC cosmological model there exists few parameters to incorporate quantum correction in general theory of relativity (GTR) of which BEC mass parameter directly relates critical temperature (T_c) of BEC which is $\leq 10^{-26}$ eV and it may be enhanced two orders considering curved space formalism. BEC model may be summarized as cold dark matter (ΛCDM) and a left over part as DE. SM and its extension predicted WIMP's like axon, sterile neutrinos (ν), graviton could be DM candidate. In this work authors revisited role of active neutrino (ν) decoupling 0.5 sec after big bang, their quantum mechanical behaviour to conditionally accept as DM particle and the BEC model with an attempt to incorporate Casimir cosmology in consistent way. The Casimir force is attractive and of quantum origin in nm scale. Enhancement of BEC mass limit is analysed.

Keywords: Bose-Einstein Condensate**,** Dark matter, Dark Energy**,** Casimir cosmology, CDM, neutrino

A2-0008

Majorana Neutrino, Torsion and Nature of Dark Matter

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Abstract

Almost 90 years back we came to know that there is predominantly excessive amount of exotic matter compared to ordinary matter. This exotic matter is nowadays termed as Dark Matter (DM) and this matter only interacts gravitationally. Its existence is understood only through its gravitational nature. The lack of experimental evidence for the non-gravitational interaction of DM may suggest that it is something beyond our current theoretical knowledge. Here we are going to study the nature of DM as that of a scalar field that originates from Bose-Einstein condensate of decoupled Majorana neutrinos in the early universe. This scalar field has been shown to assign proper dimension to the spinors through the tetrads together which represent the de Sitter boost in the SO (4,1) group. Here the axial part of torsion plays a dominant role in understanding the link between matter known from the Standard Model and the dark matter.

A2-0010

Understanding the Conductivity of Martian Environment by Using FFT Model with FDTD Method

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Abstract

We study a conductivity model of a dust devil that uses a Fast Fourier Transform (FFT) and Finite Difference Time Domain approach to analyze charging in terrestrial thunderstorms. Extensive research has been conducted on the transmission of extremely low frequency (ELF) electromagnetic waves and resonance events in the Mars atmosphere, including their impact on ionospheric dynamics, thunderstorms, and lightning. Natural electromagnetic waves generated near the surface by electrostatic discharges in dust devils could be trapped in the resonant cavity formed by the surface and lower ionosphere of mars. The lightning discharge plays an important role in the chemistry, energetics and dynamics of planetary atmospheres. The electric field is the primary cause of lightning on the Martian surface. The electric field and magnetic field in 3D can be obtained by the updated equation of time dependent Maxwell's equation.
The FFT method takes the time-domain electric field data from the calculation and converts it into the frequency domain through the electric field component [Ex]. The ion concentrations expected in lower atmosphere are not high enough to have effect on electrical conductivity. The electrical conductivity is directly calculated from electron density and collision between electrons and CO2. Our findings will be discussed further during the conference. These results and study may be useful in determining the likely lightning on Mars.

A2-0011

Nonlinearly wave-wave interaction leads to solar coronal heating.

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Abstract

Nonlinear formulation of slow Alfvén wave in magnetized plasma which can be an essential ingredient of the solar space plasma is being studied.. Various method have been adopted, mathematical formulation of the magnetohydrodynamic (MHD) waves can interpret the astrophysical phenomena happening in space plasma.The mathematical formulation of slow Alfvén wave and kinetic Alfvén wave(KAW) has been done from Maxwell equation as a make model equation. On the perturbation of slow Alfvén wave by pumped wave, the coupled wave dynamics has studied and their numerical simulation has been performed at $\theta = 50^0$. Several localized (x, z) filamentary structures have observed with diverse intensities. The spectra associated with magnetic field fluctuations are also observed with Kolmogorov scaling for inertial and dispersive range spectral index which are proportional to $k^{-5/3}$ and k^{-3} respectively.

Key words: magneto hydrodynamics (MHD) , solar corona, solar space

A2 -0012

Radiation Accretion & Rotating Black Hole Longevity in Brans-Dicke Cosmology

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Abstract

In the present study, we consider the cosmological evolution of rotating black holes in Brans-Dicke theory. We mainly discuss the effect of accretion of radiation in the early universe on black holes in Brans-Dicke theory. The rate of growth of a black hole due to accretion of radiation in Brans-Dicke theory is considerably smaller than the rate of growth of the cosmological horizon, thus making available sufficient radiation density for the black hole to accrete causally. We show that accretion of radiation by Brans-Dicke rotating black holes overrides the effect of Hawking evaporation during the radiation dominated era. The subsequent evaporation of the rotating black holes in later eras is further modified due to the variable gravitational constant, and they could survive up to longer times compared to the case of standard cosmology.

A2 -0013

Enhancing Early Warning Systems for Extreme Rainfall Events Using a Novel Cloud Detection Index: A Case Study of Mumbai, India

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Abstract

Extreme weather events, including intense rainfall, flash floods, and cloudburst incidents, have increased significantly in recent years, posing severe threats to human life, the environment, and causing global economic disruptions. Developing effective forecasting and nowcasting tools for these events is essential for safeguarding communities and ensuring efficient disaster management. This study addresses the prediction of extreme rainfall by focusing on cloud formation mechanisms and their role in precipitation.

We employed a novel Cloud Detection Index (CDI) that integrates critical atmospheric parameters, namely relative humidity and precipitable water vapor, to identify cloud presence and assess the potential for extreme precipitation. Building on the methodology of Shastri and Pathak (2019) [Advances in Remote Sensing, 8, 30–39], this research utilized CDI to detect cloud patterns associated with extreme rainfall event in Mumbai, India, several days in advance. The results demonstrate a strong correlation between CDI predictions and observed extreme rainfall, effectively identifying low- and mid-level clouds and estimating their thicknesses.

The CDI shows higher sensitivity and specificity in forecasting extreme precipitation than conventional cloud detection indices. Our findings validate CDI as a reliable early warning tool, capable of contributing to local extreme weather prediction systems. By integrating these findings with existing meteorological models, we aim to provide a more accurate framework for early warning systems to mitigate the impact of extreme weather events.

This approach offers a promising pathway for improving early warning systems, enabling proactive measures for disaster preparedness and risk reduction.

A2- 0014

CMBR Constraint on Black Hole Formation in Standard Cosmology

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Abstract

Accretion of surrounding energy-matter and the quantum mechanical Hawking evaporation are the two active ingredients for the evolution of black holes. In this work, we focus on the population of black holes in the standard cosmology scenario. We know Hawking radiation emerged from black holes can impact various astrophysical processes during the growth of the universe. One vital phenomenon among them is the distortion of the Cosmic Microwave Background Radiation (CMBR), which is the cooled remnant of the hot Big-Bang permeating entire universe and can be observed today with an average temperature of 2.725 K approximately. Considering this aspect, we have evaluated the upper limit on the initial mass fraction of the black holes in different accretion efficiencies and found quite interesting results. Moreover, we have stated the results in comparison with Brans-Dicke theory.

A2- 0015

Enhancing Solar Cell Efficiency through Down-Conversion: Current Advances and Future Perspectives

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Abstract

Solar energy is a critical component of the global transition to sustainable energy sources, yet the inherent efficiency limits of conventional solar cells often hinder their potential. This review examines recent advances in down-conversion techniques as a means to enhance solar cell efficiency. By converting high-energy photons into lower-energy counterparts that better match the absorption spectrum of photovoltaic materials, down-converting materials can significantly increase the utilization of sunlight. We explore various classes of down-converting materials, including phosphors and quantum dots, and assess their integration into different solar cell architectures. Key studies are highlighted to demonstrate the effectiveness of these approaches, showcasing improvements in power conversion efficiency and discussing the underlying mechanisms involved. Furthermore, we identify current challenges such as material stability, cost, and scalability, while outlining future research directions that could further optimize down-conversion processes. This review aims to provide a comprehensive understanding of how down-conversion can be leveraged in the quest for more efficient solar energy harvesting solutions, paving the way for next-generation photovoltaic technologies.

Keywords: Solar cell, Downconversion, luminescence materials, Phosphors

A2- 0016

Study of Photocatalytic Ability of Solvothermally Synthesized CZTS Nanocrystals in Degradation of Congo Red Dye

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Abstract

Cu_2ZnSnS_4 nanocrystals (CZTS NC) showed excellent performance in photocatalysis due to its optimum band gap and earth abundant constituent materials. CZTS NC was grown by simple, cost-effective solvothermal route which was characterized by X-ray powder diffraction (XRD), Raman spectra, transmission electron microscopy (TEM) and high resolution transmission electron microscopy (HR-TEM), UV-Vis absorption, photoluminescence (PL) and Time correlated single photon counting spectra (TCSPC). XRD analysis indicates tetragonal kesterite phase of synthesized sample which was confirmed by Raman spectroscopy and HRTEM. UV-Vis absorption study was performed to estimate band gap. Optical parameter like refractive index, extinction coefficient, real and imaginary part of dielectric constant is also determined. PL study showed the emission spectra due to presence of defect states within forbidden region. TCSPC revealed thePL lifetime which is in picosecond range. Photocatalytic activity was investigated though degradation of aqueous solution of congo-red (CR) taken as model anionic dye under irradiation of visible light and the degradation rate constant was found to be $k = 0.044\ min^{-1}$.

Keywords: Solvothermal; CZTS; Photoluminescence; Photocatalytic activity; Congo-red

A2- 0017

Insulator Waste Management for Sustainability: Potential and Practices in Construction Work in the Bikaner Region – A Review

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Abstract

The rapid development of urban infrastructure has led to increased demand for sustainable construction materials, driving a need for innovative approaches to waste management. Insulator wastes from electrical and industrial sectors, including porcelain, glass, rubber, polymer, and composite materials, presents a significant challenge due to its non-biodegradable nature. This paper explores the potential of incorporating insulator waste into brick manufacturing as a sustainable solution in the construction industry. A comprehensive review of different types of insulator waste, their material composition, and the impact on brick properties such as compressive strength, thermal insulation, and water absorption is presented. The methodology for processing and integrating insulator waste into brick production is outlined, alongside a comparative analysis of waste-incorporated bricks and conventional bricks. Findings suggest that bricks made with insulator waste offer improved strength, durability, and thermal efficiency, making them suitable for use in regions like Bikaner. This review highlights the future potential of utilizing insulator waste to enhance sustainability in construction practices.

A2-0018

New structures in radio galaxies with RAD@home citizen science, GMRT and LOFAR radio telescopes

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Abstract

Typical radio galaxies with FR I or FR II like linear structures now seem to be "tip of the iceberg" and modern sensitive radio telescopes are revealing new structures in them. Following RAD@home citizen science approach and exploring new data releases we have discovered rare new structures in radio galaxies. They have been spotted primarily using the LoTSS survey (144 MHz using LOFAR radio telescope). They include (1) a rare Collimation Synchrotron Thread" (CST) of a possibly episodic radio galaxy with a size of 600 kpc. This is only the third CST discovered, till date. (2) radio ring/swirl structures located ~100 kpc away from the AGN and at the end of the radio lobes. Only a few known so far. This is unlike the famous and puzzling "Odd Radio Circles". (3) Radio "burl" of roughly 50-75 kpc size which are located on the radio jets as compact features other than core, hotspot and kinks. (4) A few 100-400 kpc size relic lobes on one side of standard double lobed radio galaxies but the relic emission seen on only one side of the host galaxy. This is unlike the well-known double-double radio galaxies with relic lobes on either side of the young lobes. We aim to study these new-found structures in more detail by observing them using GMRT for spectral curvature imaging and aging studies. This will help us understand their role in merger and feedback driven galaxy evolution.

A2-0019

The quality of "Existence" and how the "Universe works" and deriving “The Law of Action and Consequence” and its Applications to AI

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Abstract

In this work, we explore the quality of "Existence," its mathematical value, and how the "Universe works." Our exploration leads us to understand various phenomena and the three classes of actions into which all actions fall. We also identify the controlling entity of the Universe, which governs all sentient and insentient matter. We observe an architecture in which all entities are managed by this controlling entity, which is all-pervading and responsible for creating, maintaining, and destroying both sentient and insentient objects. We find that all objects are capable of seven actions, all regulated by this controlling entity, whose role is to maintain the Universe. Additionally, we unravel "The Law of Action and Consequence" and how it governs everything in the Universe. This crucial law is key to keeping AI in check and granting it an "artificial conscience," ensuring its safety for humanity. The work answers many long-standing questions in physics by introducing the quality called “Existence”, it derives an ontology from the Sanskrit language which reduces all observed entities to four entities, such a reduction made possible this project which helps us to understand what the Universe contains?, what purpose does something serve ? and what law regulates all actions ? and what is the controller ?.

B1-0001

Pressure Sensing Dual Optical Channel by Using One Dimensional Photonic Crystal

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Abstract

Photonic crystals are periodic artificial or natural optical nano and micro devices that can control the flow of light. A theoretical model proposed for the pressure tunable dual optical channel by using one dimensional photonic crystal such as Air $[(GaAs/SiO2)^5$ $(SiO2)$ $(GaAs /SiO2)^5]$ Glass. Herein, Gallium arsenide and Silica are respectively a high refractive index material and low refractive index material with air as incidence medium and glass as substrate. The dielectric properties of the both materials are strongly variable due to the applied hydrostatic pressure. The simulation and numerical calculations are performed by using pioneer transfer matrix method. The results reflect that alteration in the pressure varies the wavelength and transmission of the both optical dual channels. Such kind of device will be most useful in optical communications where dual optical channels or wavelength sensing required.

Keywords: - Photonic crystal, Gallium arsenide, Silica, Transfer matrix method.

B1-0002

Understanding the extent of Crystal Defects in Electrical Property Degradation of MWIR HgCdTe/CdZnTe Detectors

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Abstract

Defects within epi-layers and near interfaces contribute significantly to the dark current at 77 K. An increase in dark current leads to higher dark current and hence a higher noise equivalent temperature difference (NETD), which degrades image resolution[1]. To understand diode performance, it is crucial to examine the extent of defects and their impact on carrier concentration and mobility. This paper investigates defects present at the MCT/CZT interface, their extent in the epi-layer and impact on critical electrical parameters, such as carrier mobility and concentration. The study employs advanced characterization techniques, including High-Resolution Transmission Electron Microscopy (HRTEM), Energy Dispersive Spectroscopy (EDS), and Etch Pit Density (EPD) to analyze the extent of defects from the surface of the MCT epi-layer to the MCT/CZT interface. The density of etch pits increased from 10^5 to 10^7 cm^{-2} as depth from the MCT surface increased. % IR transmission also decreased with increasing depth from the MCT surface Mobility and carrier concentration, were measured at 77 K using the Hall Effect method. The results indicated that device quality was superior when defects were localized within 1 µm of the interface. In EDS analyses, the elemental profile was found to be in precise stoichiometric order when defects were localized within 1-3 µm. Mixed behavior of carriers observed near interface. The materials in which resistivity found 4-8 ohm/cm from surface to interface, I-V characteristic of the diode found purely resistive. In contrast, device performance was categorized as good with defects situated within 3 µm, and less satisfactory when defects extended to 5 µm from the interface.

Key words: HgCdTe, HRTEM, EDS, EPD, Hall Effect, and SEM

B1-0003

Design a Hemoglobin Concentration based Biosensor using 1D Binary Photonic crystals

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Abstract

A hemoglobin concentration-based biosensor has been examined by using one-dimensional binary photonic crystals. In the proposed device a thin layer of blood sample is inserted between two alternate layers of Si/BaF_2 materials. The concentration of hemoglobin in RBC is a function of the refractive index. The sensing performance of a one-dimensional binary photonic crystal is based on slightly change in the hemoglobin refractive index/ concentrations. The transfer matrix method is employed to analyze the various properties like transmission efficiency, quality factor, sensitivity, and detection limit of a biosensor. The proposed structure exhibits excellent results with any change in the hemoglobin concentration and shows a high sensitivity of about 464.01 nm/RIU. The quality factor and detection limit of the proposed biosensor is recorded as 1419, and 1.40 $\times 10^{-3}$ RIU, respectively.

B1- 0004

Photonic Crystal Fiber-based Refractive Index Sensor for Early Cancer Detection for terahertz regime

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Abstract

This article reports a novel cancer detection sensor featuring a rectangular core Photonic Crystal Fiber (PCF) designed to identify cancerous cells in the cervix, breast, and skin. The PCF's exceptional detection capabilities allow us for the identification of cancerous cells with an efficient and precise way. COMSOL Multiphysics software based on the finite element method, was used to study and analyze the optical properties of this sensor at various values in order to achieve optimum outcomes. The frequency range of 0.9 to 3 THz in the terahertz spectrum has been investigated to achieve higher relative sensitivity with minimal confinement loss. At a frequency of 2.1 THz, significant relative sensitivity responses of 97.75%, 97.40%, and 97.93% have been obtained for cervix, breast, and skin cells, respectively. The confinement losses of x-polarized fundamental mode for cervix, breast, and skin cancer cells have been estimated as low as 2.55×10^{-15}dB/cm, 4.15×10^{-17} dB/cm, and 6.0×10^{-17} dB/cm, respectively. While, the effective mode area of 4.08×10^{-08} m^2, 4.07×10^{-08} m^2 and 4.03×10^{-08} m^2, Non-linear coefficient of 2.29×10^{-08} $W^{-1}m^{-1}$, and birefringence of 0.001327, 0.00138 and 0.001295 are obtained. This device utilizes the distinct photonic properties of cancer cells to deliver fast, reliable, and highly accurate detection methods for identifying cells in breast, cervical, and skin cancers. This sensor provides exceptional sensitivity for cancer detection. With these improved outcomes, the proposed sensor design can be effectively applied in the medical field for the early detection of cancer in the human body.

B1- 0005

Photonic Crystal Fibers infiltrated with nitrobenzene for nonlinear applications

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Abstract

This article reports three novel Photonic Crystal Fibers (PCFs) capable of assuring various critical applications such as biomedical diagnostics, explosives detection, enhanced gas sensing capabilities and improvised food quality monitoring systems. COMSOL Multiphysics software based on the finite element method, was used to study and analyze the optical properties of the proposed PCFs at various values of wavelength in order to achieve optimum outcomes. The study has been carried out in near as well as mid-infrared region with a wavelength range of 0.4 μm to 3.0 μm, to achieve relatively flat dispersion profile, minimum effective mode area and low confinement loss. Three designs with rings of air holes embedded in octagonal shape around core , 1st with silica core (#S), 2nd with circular nitrobenzene core (#N) , 3rd with elliptical nitrobenzene core with X-polarisation (#NX) & Y-polarisation(#NY) leading to birefringence has been studied . At a pump wavelength of 2.0 μm, the effective mode area of (#S) is 2.75 μm^2, (#N) is 2.19 μm^2, (#NX) is 1.97 μm^2 & (#NY) is 1.90 μm^2. Non-linear coefficient of (#S) is 33.020 $W^{-1}km^{-1}$, (#N) is 28.700 $W^{-1}km^{-1}$, (#NX) is 31.953 $W^{-1}km^{-1}$ & (#NY) is 32.981 $W^{-1}km^{-1}$. The dispersion values are found to be -33.259 ps/nm/km, 9.689 ps/nm/km, 37.940 ps/nm/km & 33.541 ps/nm/km for (#S), (#N), (#NX) & (#NY) respectively. With these improved outcomes, the proposed fiber design can be effectively employed in security applications and sensing technologies.

B1-0006

The Structural and Optical Characteristics of the series of Eu^{+3} Activated Vanadate Garnet Phosphors

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Abstract

The garnet phosphors are always earned extensive attraction due to their optical and structural properties. The garnet materials have wide range of applications. CLZVO: Eu^{3+} prepared by solid state reaction method. The emission color of the prepared sample can be easily controlled by the different composition of sensitizer. The materials were excited by ultraviolet energy. The as-prepared sample underwent various investigations like XRD, reflectance, Photoluminescence excitation and emission. The materials can be used for preparation of LEDs, optical temperature sensor, active powder in solid state laser and CRT.

Keywords: Photoluminescence, solid state reaction, garnet phosphor, temperature sensor.

B1-0007

Synthesis and Study of Optical Properties of $CdSO_4:Dy^{3+}$ Doped Yellow Emitting Phosphor For White -LED Applications

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Abstract

This article report $CdSO_4:Dy^{3+}$ phosphor which were synthesized using recrystalization method. Crystal structure and phase formation of the product was identified by powder XRD technique and partical morphology was studied by FE-SEM. According to the results of the PL analysis carried out by the Hitachi F-7000 fluorescence spectrophotometer. The photoluminescence (PL) spectra were investigated under 350 nm(UV) excitation, two emission peaks were obtained one at 483 nm, which falls under the blue region, and the other at 575 nm, which falls under the bright yellow region. These two emission peaks correspond to the $^4F_{9/2}$ to $^6H_{15/2}$ and $^4F_{9/2}$ to $^6H^{13/2}$ transitions, respectively. We suggest that the $CdSO_4:Dy^{3+}$ can be employed as an excellent luminescent material with ultraviolet radiation as an excitation source for a variety of optical applications based on its optical properties. White light for WLED applications can be produced by a special phase doping of Dy^{3+} species in the host material with yellow and blue emission.

Keyword: Yellow emitting phosphor, Re crystallization Method

B1-0008

Study of optical property of newly prepared Ce3+ doped Li15(SO4)5F4Cl unique halosulphate phosphor

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Abstract

A unique series of Ce3+ ions doped Li15(SO4)5F4Cl alkaline halo sulphate phosphors is prepared by wet chemical method first time in the history of phosphors. To determine the phase formation and purity, X-ray diffraction (XRD) studies were used. Also, scanning electron microscopy (SEM) for morphological studies and Fourier Transform Infrared (FTIR) spectroscopy which effectively identified the chemical bonds present in the molecule were performed. Photoluminescence (PL) properties of the as-prepared phosphors were investigated and the Ce3+ ions in these hosts were found to give a broadband emission in the UV range. It may serve as promising lamp phosphors in the UV range and be utilized for scintillation.

B1-0009

Quantum Efficiency Optimization in Fiber Laser Materials: The Role of Upconversion and Photodarkening

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Abstract

The quest for higher optical power in commercial laser technology drives the exploration of appropriate and durable materials for high-power fiber lasers. This study investigates a range of glass host materials—including phosphate, silicate, borate, tellurite, germanate, LaF_3, and fluorozirconate—doped with rare earth ions and optimized nanoparticles. A theoretical framework is developed to analyze the competition between radiative and non-radiative processes, which reforms the emission and absorption spectra. This framework facilitates the compositional tailoring of materials with particular emphasis on upconversion mechanisms that significantly boost quantum efficiency (QE). The non-radiative rate contributes to the observed upper state lifetime (τ), described by the equation:

$$\frac{1}{\tau} = \ w_r + \ w_{nr}$$

Trivalent ions such as Ytterbium, Erbium, and Thulium are synthesized for semi-empirical calculations within this framework. The manipulations indicate that maximizing the separation between individual atoms within nanoparticles leads to observable photodarkening. Additionally, it demonstrates that adjusting empirical parameters results in exploring fluoride crystals as host materials due to their notably low non-radiative rates. The reduction in non-radiative rates for trivalent ion dopants also enhances QE and strengthens ion-host interactions. This phenomenological analysis provides insights into concentration quenching effects in nanoparticle dopants.

Key Words: Photodarkening, nano particles, ion-host interaction, quantum efficiency, upconversion.

B1-0010

Si-based one-dimensional photonic crystal as a selective optical filter in THz frequency region

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Abstract

This study investigates the transmission properties of a SiO2/Si bilayer system, focusing on the creation of bandgaps in the THz frequency range within one-dimensional photonic crystals. These bandgaps function as barriers that prevent specific frequencies of light from passing through the crystal, allowing precise control over the transmission and reflection of THz waves. By adjusting factors such as efractive index contrast and layer thickness, bandgaps can be engineered to meet the needs of THz applications. The Transfer Matrix Method (TMM), a reliable umerical approach, is utilized to analyze the optical behavior of one-dimensional photonic crystals. The study examines how parameters like the angle of incidence, layer thickness, refractive index contrast, and the number of unit cells affect the transmission spectra. These findings offer valuable insights for the design of narrow-band optical filters for optical devices. Additionally, the results suggest the potential to design an optical filter that operates independently of the number of unit cells, enhancing its flexibility and range of applications.

B1-0011

Defect-Induced One-Dimensional Photonic Crystals: Fabrication and Characterization

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Abstract

In this study, a one-dimensional (1D) photonic crystal was fabricated using a sol-gel approach to deposit alternating layers of TiO2 and SiO2 on a glass substrate via spin coating. The structure, consisting of 5.5 bilayers, was designed to act as a Bragg reflector with each layer meeting the λ/4 condition for constructive interference. Reflectance spectra of individual TiO2 and SiO2 layers were analysed using UV-Vis spectroscopy to verify their optical properties. Subsequently, silver nanoparticles (AgNPs) were synthesized via laser ablation and incorporated as a defect layer within the 1D photonic crystal structure. The geometric thickness of the silver layer was tailored to λ/4n to induce localized optical effects within the photonic crystal. Nonlinear optical behaviour of the AgNps was investigated using single beam open aperture z-scan technique. This analysis provided insights into the nonlinear absorption properties, crucial for potential applications in photonics. Furthermore, theoretical simulations were conducted using the software COMSOL Multiphysics to predict the reflectance and transmittance spectra of both the pristine photonic crystal and the defective structure with AgNps. Additionally, the electric field profile of the photonic crystal Bragg reflector was simulated to understand its optical behaviour in detail.

Overall, this comprehensive experimental and theoretical approach offers a deeper understanding of the optical characteristics and potential applications of 1D photonic crystal with defect layers, paving the way for advancements in optical devices and systems.

B1-0012

Fundamental Analysis of TMM and PWEM in One-Dimensional Photonic Crystals: Advantages and Limitations

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Abstract

This research provides a fundamental analysis of the Transfer Matrix Method (TMM) and Plane Wave Expansion Method (PWEM) for one-dimensional photonic crystals. We evaluate their effectiveness in computing band structures and transmission spectra, highlighting TMM's computational speed and efficiency in complex layer configurations, while noting PWEM's precision in band gap characterization, albeit at a higher computational cost. By examining the advantages and limitations of both methods, this study lays the groundwork for optimizing photonic device design and underscores the importance of robust computational techniques in advancing photonic crystal applications in modern optics.

B2- 0002

A Review of Investigating Open Heavy-Flavour Production via elliptic flow in Collision Systems with ALICE at the LHC

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Abstract

The quark–gluon plasmonic state (QGP) established during ultra-relativistic heavy-ioncollisions can be extensively studied using heavy quarks as vital probes. The contention centers on the most recent upshots from the ALICE Collaboration dealing with open heavy-flavour creation in proton-proton and lead–lead impacts. Quantifications of the emergence of openheavy flavors in lead–lead impacts are indispensable to comprehend the heavy-quark transport mechanisms and energy loss in the plasmonic state. In-depth apprehension regarding heavy-flavour particles' function within the medium's collective behaviour, the path-length reliance of their in-medium energy drop, and viable rearrangement consequences amid hadronization can be procured by reviewing their elliptical effluence ($v2$) coefficient. Open heavy-flavour creation imparts a benchmark for assaying perturbative quantum chromodynamics projections and gauging blazing hot-medium aftermaths in heavy-ion impacts in diminutive hadronic setup such as proton-proton.

B2- 0003

Decay Properties of Charmed B Mesons

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Abstract

To elucidate the confining interaction experienced by the free relativistic independent quarks within the meson, we utilize a phenomenologically derived potential that is not dependent on quark flavor. This potential is expressed as a combination of scalar and vector parts in a square root form. Corrections for the spurious center of mass motion and other residual interactions are accounted for when calculating the meson mass spectra using a perturbative approach. Examples of such interactions include single-gluon exchange over small distances and quark-pion coupling due to restored chiral symmetry. Using the same potential parameters, we calculate mesonic decay of B- mesons, rare decays of B^0, B_S^0 mesons. The estimated results of mesonic, and rare leptonic decay widths of charmed B mesons are close to some theoretical model like LQCD, and experimental predictions. Finally, we also calculate the mixing parameters of $B\ and\ B_S-$ meson oscillations. The results for mass oscillations, Δm (mass difference) and other mixing parameters such as $x_q, y_q\ and\ \chi_q$, of $B^0$and B_S-meson shows excellent agreement with some theoretical model calculations and PDG results.

Key Words: Mesonic Decay widths, Rare Decay widths and its Branching Fractions and Mixing Parameters of $B^0$and B_S Meson.

B2- 0004

Grand Unified Theory and Unification of Fundamental Interactions of Quaternion-Octonion

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Abstract

Grand unified theories are discussed accordingly in terms of Quaternion and Octonion in terms of quaternion basis elements and Pauli matrices as well as the Octonion and Gell-Mann matrices. Connection between the unitary group of GUT's and normed division algebra has been established to redescribe the $SU(5)$ gauge group. The $SU(5)$ gauge group and its subgroup $SU(3)_C \times SU(2)_L \times U(1)$ have been analyzed in terms of quaternion basis elements.

Keywords: Quaternion, Octonion, QCD, Grand unified theory.

B2- 0005

Investigating the mass spectra of all strange tetraquark in Quadratic Quark Confinement

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Abstract

Over the past two decades, numerous states containing multiple strange quark resonances have been experimentally observed. In this study, the mass spectra for strangeonium mesons, strangeonium diquarks, and all-strange tetraquarks are computed using semi-relativistic framework. These computations include relativistic mass corrections and employ a Quadratic quark confinement. The study concludes by offering predictions for various states as potential candidates for resonances such as X (2370), $f_0(2200)$, and others, alongside comparisons with other theoretical models and the two-meson threshold.

B2- 0006

Exploring the heavy-light pentaquark in Hyper-central Constituent Quark Model

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Abstract

In this study, we examine the mass spectra of heavy-light pentaquarks using the Hyper-central Constituent Quark Model (hCQM) within the framework of the non-relativistic quark model. For heavy-light pentaquarks, we calculate the ground-state masses containing charm and beauty quarks for various J^P values. This is accomplished using two different confining potentials, along with an enhanced form of hyperfine interaction. The mass spectra for these pentaquarks are computed across multiple states, including S, P, and D waves, with corresponding spin-parity assignments. Additionally, Regge trajectories are explored for various states to confirm the consistency of the results. Finally, the calculated pentaquark masses are compared with experimental data and other theoretical predictions.

B2- 0007

Investigating the mass spectra of di-hadronic molecule by potential model

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Abstract

In this study, we tackle the intriguing challenge of identifying and understanding the interactions governing hadronic molecules. To compute the mass spectra, we employ the One Boson Exchange potential combined with a Yukawa-like screened potential in their relative s-wave state. We propose that two color-neutral hadrons interact through a dipole-like interaction, leading to the formation of a hadronic molecule. To distinguish these molecules from other hadronic states, we apply Weinberg's compositeness theorem. Using the suggested interaction potential, we calculate the mass spectra for various di-mesonic states, including ππ, ηη, φφ, and J/ψ J/ψ.

B2- 0008

Magnetic moment of heavy flavoured baryons

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Abstract

The magnetic moment is a fundamental intrinsic property of particles that provides deep insights into their internal structure and the dynamics governing transition processes during decay modes. As a result, the study of the electromagnetic properties of baryons has become a crucial area of both theoretical and experimental research. Over the past few decades, significant progress has been made in identifying the heavy baryons, contributing to a better understanding of their behaviour. In the present study, we focus on singly heavy-flavour baryons, specifically analysing their electromagnetic properties. We compute the magnetic moments of the ground state baryons with $J^P = \frac{1^+}{2}$ and $\frac{3^+}{2}$. additionally, we provide a comprehensive comparison of our predictions with those obtained through various other theoretical approaches. This comparative analysis highlights the consistency and differences between our results and existing literature, offering a broader perspective on the ongoing investigations in this field.

B2- 0009

A Comprehensive Study of Mass Spectra of Ξ_{cb} and its Properties using hCQM

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Abstract

In the current study, we explore the properties of the doubly heavy baryon Ξ_{cb} using the Hyper Central Constituent Quark Model (hCQM). Our calculations focused on determining the masses of both the ground state and excited states ofΞ_{cb}. To enhance accuracy, we incorporated higher-order corrections, including second-order corrections in mass within the context of spin-dependent terms. This enabled us to precisely determine the correct order of spin splitting. We have successfully determined the spin-parity J^p for ground and excited states, providing insights into the quantum nature of the Ξ_{cb} baryon. Furthermore, we have done a comprehensive comparison with our predicted resonance masses of Ξ_{cb} and compared it with other theoretical approaches, providing a comprehensive understanding of its properties.

B2- 0009

Investigating the mass spectra of Tetraquarks using Regge Phenomenology

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Abstract

This work investigates the mass spectra of tetraquarks in the light sector using Regge Phenomenology, considering tetraquarks as composed of diquark-antidiquark pairs. We employ a quasi-linear Regge trajectory ansatz in the (J, M^2) plane, where J represents the total angular momentum and M denotes the mass. The model integrates the principles of additivity for both the intercepts and the inverse slopes of the Regge trajectories across different quark flavors. By focusing on light quarks, we aim to provide a comprehensive understanding of the tetraquark states, identifying their behavior in terms of angular momentum and mass. The equations used for the additivity of intercepts and slopes provide a novel approach to constraining the dynamics of the light quark sector, leading to more accurate predictions of the mass spectrum. Our results are expected to shed light on the underlying dynamics governing tetraquarks, offering new insights into their structure and contributing to ongoing discussions on exotic hadrons.

B2- 0010

Exploring Ω_c baryon states within the relativistic flux tube model

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Abstract

Recent advancements in experimental facilities have enabled the direct observation of numerous single-charmed baryons. Inspired by the LHCb's recent observation of five narrow excited states of Ω_c^0 baryon in the $\Xi_c^+ K^-$ channel named $\Omega_c(3000)^0$, $\Omega_c(3050)^0$, $\Omega_c(3065)^0$, $\Omega_c(3090)^0$, and $\Omega_c(3120)^0$, we study the mass spectra of Ω_c^0 baryon with its quark diquark structure. The spin average mass is computed within the framework of the relativistic flux tube model using the modified Regge relation between mass and angular momentum. Furthermore, we take into account the effects of spin-dependent interactions. The analysis revealed a good agreement between the predicted values and the existing experimental data, which greatly helped predict spin-parity assignments for the states that were observed in the experiments.

B2- 0011

Study of the strong decay of Λ_c and Ξ_c baryons

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Abstract

Significant advancement has been made in recent years in our knowledge of the properties of charmed baryons [1]. In this work we study the strong decay of Λ_c and Ξ_c baryons within the framework of Heavy Hadron Chiral Perturbation Theory (HHChPT), which synthesizes a chiral and heavy quark symmetry [2]. We compute the strong decay width of $1P$ states of Λ_c and Ξ_c baryons. Spin parity quantum numbers of $\Lambda_c(2593)$, $\Lambda_c(2625)$, $\Xi_c(2790)$, and $\Xi_c(2815)$ states have not been measured experimentally yet but it is expected to be $\frac{1}{2}^-$, $\frac{3}{2}^-$, $\frac{1}{2}^-$, and $\frac{3}{2}^-$, respectively. These estimated spin-parity assignments are supported by our computed decay widths, which correspond closely with the experimentally measured width.

B2- 0012

A Comprehensive Study of Mass Spectra of Ξ_{cb} and its Properties using hCQM

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Abstract

In the current study, we explore the properties of the doubly heavy baryon Ξ_{cb} using the Hyper Central Constituent Quark Model (hCQM). Our calculations focused on determining the masses of both the ground state and excited states of Ξ_{cb}. To enhance accuracy, we incorporated higher-order corrections, including second-order corrections in mass within the context of spin-dependent terms. This enabled us to precisely determine the correct order of spin splitting. We have successfully determined the spin-parity J^p for both ground and excited states, providing insights into the quantum nature of the Ξ_{cb} baryon. Furthermore, we have done a comprehensive comparison with our predicted resonance masses of Ξ_{cb} and compared it with other theoretical approaches, providing a comprehensive understanding of its properties.

B2- 0013

Indirect Signature of quark gluon plasma in high magnetic field

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Abstract

Using a phenomenological model of quark-gluon plasma (QGP), our work examine into thermodynamic parrameter to explore the properties of QGP matter in the presence of a highly magnetic field, supposed to be generated at BNL and CERN. It is now confirmed that the substantial high magnetic fields exists in heavy-ion collisions. We consider both static as well as dynamic part of high magnetic fields within the QGP medium. The existence of a magnetized field in QGP medium proves significant change in the properties of QGP medium. Our exploration focuses on the QGP equation of state (EoS) in the presence of high magnetic field, and the obtained results are systematically compared with other theoretical results. We address some of key aspects of QGP in order to predict the phase transitions. Notably, the results are instrumental, particularly in the vicinity of high temperatures and under the influence of highly intense magnetic fields. These results could be significant for the future research in the heavy ion collisions and quark gluon plasma.

B2- 0014

Multiplicity Distributions of Photons from Heavy Ion Collisions

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Abstract

Study of Particle multiplicity as functions of the colliding system and energy provide important constraints on the initial conditions of the matter created at the early stage of reaction. The scaling behaviour of particle production carries information on the reaction dynamics. As many experimental signatures in heavy ion collisions require a comparison of observables for different system sizes. The observation of a new phase of strongly interacting matter, the quark-gluon plasma (QGP), is one of the most important goals of current nuclear physics research. This analysis shows that the distribution of nuclear fragments stripped in contacts of projectile with different target nuclei have different probability distributions. The results of this investigation demonstrate how heavily these distributions depend on the mass of the target nucleus in terms of the total charge of the spectator fragments.

B2- 0015

Magnetic Strange Quark Matter with Thermal Mass

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Abstract

The primary goal is to calculate the thermodynamic properties of strange quark matter in the presence of a magnetic field using a theoretical approach. By applying a quasiparticle model, we enhance our capability to determine the equation of state for strange quark matter under intense magnetic fields. This quasiparticle framework allows us to examine the equation of state and investigate the properties of strange quark stars across varying magnetic field strengths, considering all relevant factors.

B2- 0016

Expansion of QGP droplet in the early universe

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Abstract

We use a phenomenological model to study the expansion of a quark-gluon plasma (QGP) droplet in the early universe. Using a quasiparticle model, we employ the Friedmann approach to derive the equation of state for QGP. Studies considering zero chemical potential during early universe exist, however studying the behaviour of the QGP droplet at non-zero chemical potentials during the setting of early universe is challenging and less explored. Our analysis explores temperature and other thermodynamic observables at non-zero chemical potential. This inclusion is crucial, as it significantly influences the variation of thermodynamic variables over time. This study yields valuable insights into understanding the dynamics of QGP during the early formation of the universe in the presence of a chemical potential.

B2- 0017

Strange quark matter in the presence of intense magnetic field

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Abstract

In this study, our aim is to calculate thermodynamic observables for strange quark matter when subjected to a magnetic field, employing a quasiparticle approach. We introduced a simple model, aimed at facilitating the computation of the equation of state for strange quark matter under the influence of a strong magnetic field. Subsequently, employing the quasiparticle approach, we investigate the equation of state to examine various properties of strange quark stars under varying magnetic field strengths, incorporating appropriate factors for its analysis. Therefore, our results are useful in order to explore fascinating properties of strange quark matter.

C1- 0001

Impact of Active Layer Thickness variations on the performance of P3HT: PCBM -Based Organic Solar Cell

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Abstract

In this study, we investigated hybrid bulk heterojunction organic solar cells composed of poly (3-hexylthiophene) (P3HT) and phenyl-C61-butyric acid methyl ester (PCBM). The reference cell, containing a P3HT: PCBM active layer sandwiched between ITO/PEDOT: PSS and ZnO/Al electrodes, exhibited higher efficiency. By varying the active layer thickness, we observed an improved fill factor (FF), demonstrating that optimizing the thickness of the P3HT: PCBM layer controls the short-circuit current density (J sc) of hybrid solar cells, while ZnO nanolayers improve the open-circuit voltage (V oc) of organic solar cells. Using FLUXIM-SETFOS software, our study aims to maximize the fill factor and power conversion efficiency of P3HT: PCBM-based organic solar cells (OSCs) by adjusting the thickness of the P3HT: PCBM layers. Our results show that J-V characteristics are influenced by layer thickness variations and that power conversion efficiency can be enhanced by optimizing these thicknesses, with simulations indicating an optimal active layer thickness that yields the highest fill factor and power conversion efficiency. Simulation results reveal that the optimum thickness for the active layer, P3HT: PCBM is 150 nm, with 5.72% power conversion efficiency.

C1- 0002

Effective Electrical Conductivity of High-Density Polyethylene Composites with various metal fillers: A Short Review

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Abstract

Over the past few years, conductive polymer composites have gained considerable interest due to their potential uses in a variety of areas, such as antistatic systems, electromagnetic shielding, semiconductors, corrosion-resistant coatings, drug delivery systems, and batteries. This review highlights research findings on the electrical conductivity of High-Density Polyethylene (HDPE), which is conventionally considered an insulator. But when filled with various fillers including Carbon based filers, metal powders, metal oxides, recycled ground tire rubber, cellulose fibers etc. results in the electrical conductive composite. The effect of fillers (e.g. type and size), the use of metal fillers, is deeply studied. A maximum conductivity of 2.2×10^{5} S/Cm is observed with Ni filler at a very low filler content of 5-10 vol. % whereas least electrical conductivity of 1.18×10^{-11} S/Cm is observed for Al fillers also, percolation extends in a wide range of 5-30 vol. %. Here we have discussed various references to the recent studies on the product and performance.

Keywords: HDPE, Effective electrical conductivity, different fillers, volume fraction

C1- 0003

Polymer doped NiO blend composite for electrochemical performance

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Abstract

Solution casting technique was used to prepare of Polymer and polymer/NiO blends films. The surface morphology displayed homogeneous dispersion of NiO on the Polymer matrix, the formation of the NiO phase in the polymer, displaying a sphere nature that could potentially enhance the materials, Additionally, Atomic Force Microscopy (AFM) was utilized to analyze the chemical interactions and variations in surface roughness present in the Polymer blend film, along with different weight percentages (wt%) of NiO-loaded composites. while the LSV curve exhibited a linear shape across different scan rates from 10 mV/s to 50 mV/s. The Polymer /NiO loaded polymer blend films showcased synergistic properties contributing to enhanced electrochemical performance.

C1- 0004

Synthesis and NLO Investigations of Rhodanine-Thiophene Oligomer by Hyper-Rayleigh Scattering and Z-Scan Analysis

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Abstract

A new type of nonlinear optical oligomer RO1 containing 3-ethyl-rhodanine as the acceptor moiety was attached with thiophene donor unit was synthesized. This facile structural positioning of the donor and acceptor unit leads to fine tune the photophysical, thermal and NLO properties was systematically examined in this work. New NLO oligomer was synthesized with the help of the Stille coupling reaction. For studying structure-property relationship, the oligomer was characterized with structural, physical, electrochemical, optical, and theoretical studies etc. The current oligomer gives better solubility and thermal stability, which is suitable for optoelectronic applications. Density functional theory studies were calculating the HOMO-LUMO energy levels and understanding the in-depth structural characteristics of the oligomer. The oligomer gives a broad emission band in the UV-Visible region between 300 nm to 600 nm and the solvatochromic study confirms the positive solvatochromic behavior of the oligomer. The morphology study by using a scanning electron microscope reveals the distinct morphological characteristics of the oligomer. Second-order NLO properties such as, the first hyperpolarizabilities, β value and static hyperpolarizability, β_0 value were evaluated from Hyper-Rayleigh scattering (HRS) method and the oligomer gives high β value using a standard wavelength at 1064 nm. Third- order NLO properties gained from open-aperture Z-Scan measurements with 5 ns laser pulses at 532 nm disclose an optical limiting behavior of the oligomer due to three- photon absorption.

Keywords: Rhodanine (Rh), Nonlinear optics (NLO), Density Functional Theory (DFT), Hyper-Rayleigh scattering (HRS), Z-Scan analysis.

C1- 0005

Influence of lead-free BCZT ceramic filler on the dielectric, ferroelectric and energy storage characteristics of PVDF-TrFE based polymer composite film

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Abstract

The work represents PVDF−TrFE+BCZT two-phase composites with detailed analysis of the dielectric, ferroelectric, and energy storage properties. BCZT ceramics prepared by cost effective mixed oxide method were added to PVDF-TrFE solution with different weight percentages for fabrication of composite films by solvent casting followed by hot pressing method.The presence of more than 70% of electroactive β-phase in the composites is calculated from FTIR study. The room temperature dielectric constant of the pure polymer increases gradually upon the addition of ceramic filler. The strong interaction between the P(VDF-TrFE) matrix and BCZT particles at the interface may be the cause of this remarkable improvement in the dielectric characteristics. The ferroelectric and energy storage properties of the composite films are discussed from room temperature hysteresis (P-E) loops. The energy storage efficiency of the composite samples is more than 70% suitable for energy storage applications.

Keywords: P(VDF-TRFE), Polymer Ceramic Composite, Dielectric Properties, Energy Storage density.

C1- 0006

Conduction mechanism of the PVC-PMMA Polyblend films

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Abstract

The electrical conduction mechanism of blend film (PVC and PMMA) has been studied at various temperatures in the range 313K to 353K. The results are presented in the form of I-V characteristics. Analysis has been made in the light of Poole-Frenkel, Fowler-Nordheim, Schottky, Ln(J) versus T plots, Richardson and Arrhenius plots. Results analysed suggest that, Schottky-Richardson mechanism is primarily responsible for observed conduction.

Keywords: Polyblend film, Conductivity.

C1- 0007

Synthesis & characterization of PMMA/$SrAlO_7Eu^{2+}Dy^{3+}$ Polymer Electrospunn fiber

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Abstract

PMMA/$SrAlO_7Eu^{2+}Dy^{3+}$ nanofibers were prepared by electrospinning method. 2gm PMMA was dissolved in 10ml of DMF solvent to give mass fraction of 50wt% and magnetically stirred (150 to 250 rpm) for 5hr at room temperature. Then 2gm of Eu, Dy doped Strontium Aluminates was added to uniform solution and stirred for 16 hrs. with magnetic stirrer till homogeneous at room temperature. The homogeneous solution was then transferred to the 5ml plastic syringe to produce the nanofibers from the electrospinning machine. The distance between the needle and the metallic collector was 15 to 16cm. the flow/feed rate was kept at 3ml/h and high voltage was maintained at 18-20kilovolt. The metallic collector is rotated with the speed of 1200 to 1400 rpm so as to collected uniform sheet of the PMMA/$SrAlO_7Eu^{2+}Dy^{3+}$ polymer fibers. Scanning electron microscopy (SEM), FTIR and X-ray-diffraction (XRD) analyses revealed that the morphology of the PMMA/$SrAlO_7Eu^{3+}Dy^{2+}$ nanofibers consist of the dispersion of $SrAlO_7Eu^{3+}Dy^{2+}$ nanoparticles with monocyclic structure in PMMA nanofibers. Excitation of phosphors with UV light (320 nm) produced emission spectra at λ= 520 nm for $SrAlO_7$:Eu,Dy showing bright sea green luminescence The prepared nanofiber is applicable in the field of smart clothing, wound dressing, luminescent fabric designing, etc.

C1- 0008

Effect of Salt and Charge Density on the Dynamics of Acrylamide-co-Sodium Acrylate Hydrogel

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Abstract

We have investigated the diffusion dynamics in the charged gel matrix using dynamic light scattering measurements. Acrylamide-co-sodium acrylate was taken as the sample for polyelectrolyte gel with different charge densities, and the effect of salt on diffusion dynamics was explored. Due to the non-ergodic behavior of the sample, the direct ensemble averaged method was employed to obtain the correlation data. All the correlation curves were fitted with adequate accuracy by single plus stretched exponential functions from which the relaxation times corresponding to fast and slow relaxation modes were acquired. Ideally, the fast relaxation is connected to the cooperative diffusion of the gel network, while the slow relaxation is related to the cluster dynamics. Since the slow mode is linked to the stretched mode, i.e. the stretched exponent, β, has a value between 0 and 1, the mean relaxation time corresponding to the cluster dynamics was calculated from the slow relaxation time. Nearly one order of difference in magnitude was seen in two relaxation times corresponding to fast and slow modes for each studied sample. As we increase the charge density of the hydrogel sample without adding salt, an increase in fast relaxation time is noticed. However, when the samples were prepared with the addition of monovalent salt, a reverse trend was detected. Here, the fast relaxation time gradually decreases, implying that the gel network becomes more diffusive. For these samples, similar behavior is also seen for the mean relaxation time.

C1- 0009

A Comparative Dynamic Analysis of Agar-Polyacrylamide Double Network Hydrogel with its associated Single Network Hydrogels

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Abstract

A mixed agar/polyacrylamide (PAM) double network (DN) hydrogel was synthesized using one-pot, heating-cooling photo-polymerization method along with its corresponding single network (SN) hydrogel of agar and PAM. The agar hydrogel was prepared by simply heating the solution followed by cooling it to room temperature, whereas the PAM hydrogel was formed with the help of photo-polymerization. Dynamic light scattering measurements were performed on the prepared samples to examine and compare the change in dynamics of double network hydrogel with its connecting independently prepared single network hydrogels. Being non-ergodic in nature, direct ensemble average approach was used to analyse the correlation data. Both the DN along with the SN hydrogels shows bimodal relaxation, where the fast relaxation is coupled to the cooperative diffusion which describes the dynamics of polymer networks and slow mode represents cluster relaxation. For all the studied samples of prepared hydrogels, there is at least an order of magnitude difference between the fast and slow mode relaxation. It has been observed that the magnitude of both the fast and slow mode relaxation time is the maximum for the DN hydrogel as compared to the SN hydrogel of either agar or PAM. The scattering experiments showed the presence of an atypical slow relaxation mode in case of DN gel. This could be as a result of more effective cross-linking from both the networks in the case of double network hydrogels.

C2- 0001

Analysis of Level Scheme of 139Pm using γ-γ coincidence method

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Abstract

This study presents an analysis using the γ-γ coincidence technique for identifying new γ-transitions of 139Pm. The technique based on time correlation between γ-rays in a cascade and ensures to observe at least two γ-rays within a time window of ±400 nanosecond. The present work reveals a significant insight into the level scheme of 139Pm. 139Pm is the nucleus of interest as it belongs to transitional A ~ 130 mass-region. The mass-region is predicted to exhibit notable and complex nuclear shapes and transitions, including triaxial shapes and varieties of shape evolution due to presence of valence particles into high-j orbitals

The transition from prolate to oblate shape was predicted for Nd, Sm and Gd nuclei at N = 78 in ref. [1]. These recent observations provide a further challenge to the theoretical models to explain the role of high-j orbitals on the evolution of different nuclear shape and riaxial−deformation. The 139Pm nucleus has been extensively studied for its high-spin states. The band structures of 137Pr, 138Nd, 139Pm and 141Eu nuclei, having neutron number N = 78, are of particular interest for the study of shape evolution and triaxial deformation due to the availability of g7/2, d5/2 and h11/2 orbitals near the proton and neutron Fermi surfaces [2-5].

C2- 0002

A Comprehensive study of Classical Liquid Drop Model of Nucleus and Modified Macroscopic Liquid drop model

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Abstract

This study focuses on solving and testing the binding energy formulation presented in *refs.* and comparing it to available experimental binding energy data for nuclei. Specifically, the work addresses the Modified Macroscopic Liquid Drop Model. The classical Liquid Drop Model, which uses the semi-empirical mass formula, offers a simple and intuitive explanation for nuclear binding energy. However, it fails to adequately account for phenomena such as magic number nuclei and fission barrier formation. The modified Macroscopic Liquid Drop Model discussed in introduces updated terms, including curvature corrections and a separate A^0 term, by treating nucleons as a gas moving along the nuclear surface. In this study, we aim to verify the claims made in the original paper and refine the fitting parameters to provide a more accurate and improved model of nuclear structure.

C2- 0003

Application of deep neural network to predict GDR cross-sections of Zr isotopes

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Abstract

The investigation of Giant Dipole Resonance (GDR) parameters plays a key role in enhancing our comprehension of nuclear structure and the behavior of heavy nuclei. The GDR mechanism dominates the photo-absorption cross-section up to 30 MeV, where the cross-section typically exhibits one or more Lorentzian peaks, depending on the deformation of the nucleus. Traditionally, GDR parameters such as centroid energy, and width are derived from experimental observations or theoretical calculations. In this study, we introduce a method for predicting the GDR parameters of the ^{90,91,92,94}Zr isotopes using a deep neural network (DNN). A comprehensive dataset, compiled from experimental GDR parameters across various nuclei, is processed and utilized to train the predictive model. The neural network is fine-tuned to achieve high accuracy and reliability in predictions. The resulting GDR cross-sections, computed from the predicted parameters, are compared with experimental results, demonstrating strong consistency within the bounds of experimental uncertainty. This predictive framework has the potential to extend to other heavy and underexplored nuclei, offering new perspectives on nuclear structure and dynamics.

C2- 0004

Applicability of VMI Model for A=130 Superdeformed nuclei

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Abstract

Our analysis is focused for the analysis of Superdeformed (SD) bands available in the mass region 130, by employing modified Variable Moment of Inertia (VMI) model for the comprehensive examination of band head spin and subsequently the level spins. The experimental data is limited for these bands so our model primarily aims to deduce the band-head spin. This approach helps us to yield quantitative results for γ-energies as well as spins across all observed bands. To ensure the accuracy of band-head and level spins, we validated our findings using the Ratio of Transition Energies over Spin (RTEOS). Notably, we observed a strong correlation between calculated and observed transition energies confirms the reliability and precision of our approach. A key outcome of this study is the prediction of band-head spins and level spins for 130 mass region Superdeformed bands. These findings help resolve the uncertainties surrounding level spins, structure of bands and identical bands, providing valuable insights for future research in this area.

C2- 0005

Shell Model Calculation of Spectroscopic Properties of 124Xe and 130Ba Nuclei for positron emission mode

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Abstract

Double beta decay (DBL)) is clear sign of new physics beyond the standard model. Depending on the relative number of protons and neutrons in a nucleus, the three additional possible processes are double electron capture (ECEC), double positron decay (β+β+) and positron emitting electron capture (ECβ+). These three processes are energetically competing and are referred as positron double beta decay (e+DBD) modes. While DBD has been observed in about a dozen nuclei, the e+DBD modes continue to be an elusive. The study of these modes require the knowledge of nuclear transition matrix elements (NTMEs), therefore, in this work, we have considered the nuclei namely 124Xe and 130Ba, and studied their spectroscopic properties such as yrast energies, quadrupole moment (Q), magnetic moment (μ) and reduced transition probabilities B(E2). The obtained values are then compared with available experimental data to check the reliability of the wave functions. These wave functions may then be used for calculation of NTMEs for these (e+DBD) modes.

C2- 0006

Isotopic Decay Analysis of Hg Nuclei Produced in Heavy-Ion Reactions

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Abstract

Nuclear reactions induced by heavy ions constitute a rich field of study, offering insights into the formation and subsequent decay of compound nuclear systems. Within this domain, the investigation of 194,196,198Hg* nuclei, produced via 12C + 182,184,186W reactions represent an ideal case for investigation. These mercury isotopes hold significant value in diverse fields including nuclear energy production, astrophysics, and fundamental nuclear structure studies. Here in the present work, we aim to conduct a comprehensive analysis of decay cross-sections for 12C + 182,184,186W reactions within the collective clusterization approach of Dynamical cluster-decay model (DCM) [1]. Specifically, we investigate the total decay cross-sections, which include contributions from both evaporation residues (σER) and fission fragments (σfiss), across a center-of-mass energy range of 48 to 78 MeV, traversing the Coulomb barrier. This highly asymmetric reaction channel is chosen based on experimental data from Ref. [2]. Our findings demonstrate a good agreement between the calculated ER cross-sections and experimental data, while σfiss remain negligible across the studied energy range. However, as excitation energies exceed 78 MeV, the contribution from fission becomes increasingly significant. A detailed analysis has been conducted using the DCM, with emphasis on preformation and penetrability factors. Additionally, an attempt is also made to investigate the role of energy dependence on the fission mass distributions of the considered nuclei.

C2- 0007

Study of ^{23}Mg (p, γ) ^{24}Al astrophysical reaction

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Abstract

^{23}Mg (p, γ) ^{24}Al reaction is known to be a potential means for breaking out of the Ne-Na cycle to heavier nuclear species in explosive hydrogen-burning stellar environments such as novae, type I X-ray bursts and accreting black holes. It also plays a key role in linking the Ne-Na and Mg-Al cycles in O-Ne classical novae. However, at temperatures, T > 1 GK, the ^{23}Mg (p, γ) ^{24}Al reaction becomes less important because production of ^{23}Mg is bypassed on the proton-rich side. In this paper, we aim to calculate the stellar reaction rates theoretically in the temperature range 0.1 < T < 1.0 GK with minimum inconsistencies. In case of unstable nucleus like ^{24}Al production, the experimental database is scarce. Therefore, theoretical research is equally crucial for improving the estimates of the overall reaction rate. Energy levels of unstable isotope ^{24}Al and γ-ray partial widths for astrophysically important resonances are derived using Shell Model calculations via NuShellX code. We identified an essential resonance state that appeared to contribute considerably to the reaction rate; its energy level, which we determined to be 2345 keV, fits perfectly with the energy reported by G. Lotay et al. (2008) in the experiment. The gamma width (Γ_γ) of this resonance state is also in good agreement with the value reported by Herndl et al (1998). The work involves determining proton partial width, calculating the S-factor at Gamow energy, and assessing the reaction rate to understand its impact on nucleosynthesis for elements with A > 20.

C2- 0008

Determination of Erc.m. = 107 keV resonance strength (ωγ) of 25Mg (p, γ) 26Al astrophysical reaction using shell model calculation

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Abstract

The discovery of the 1.809 MeV gamma-ray in 1984 by Mahoney et al. using the HEAO-C satellite provides proof that 26Al nucleosynthesis is currently occurring in the Galaxy. The primary process in the galaxy for producing 26Al is 25Mg (p, γ) 26Al, and the capture reactions of isolated narrow resonances in the excited state of 26Al dominate its astrophysical reaction rates. Levels between Erc.m. = 50 keV and 310 keV are more significant in the investigation of galactic 26Al as the temperature range of astrophysical interest is T = 0.02 - 2 GK. Since 1970, several experiments have been conducted to investigate the 25Mg (p, γ)26Al reaction. However, because of the small cross section and significant background effects of cosmic rays, direct observations on Earth's surface are limited. Here, we have determined Erc.m. = 107 keV resonance strength (ωγ) of 25Mg (p, γ) 26Al astrophysical reaction using shell model code NuShellX. We have utilized the sd model space and the USDB interaction to reproduce the excited states of 26Al. Theoretically, the resonance state has been reproduced at Ex = 6361 keV (Eexpt. = 6414 keV) within only 53 keV energy difference. After that, the proton width (Γp) and spectroscopic factor (C2S) have been calculated. Finally, we have estimated the resonance strength (ωγ), i.e, equal to 2.75 X 10-11 eV, which is in excellent agreement quoted by J. O. Fern´andez Niello et al. The outcome serves as a guide for the future 25Mg (p, γ) 26Al direct measurements.

C2- 0010

Effect of centrifugal potential on p-emission from 183W* nucleus formed in n-induced reaction

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Abstract

Charged particle emissions from nuclei populated in asymmetric incoming channel such as neutron induced channels have gained interest from nuclear scientists and engineers as they help to understand the nuclear behavior, structure and stability. In this context, the p-emission from 183W* nucleus populated in n+182W reaction is investigated within the Dynamical Cluster-decay Model (DCM) [1], in reference to the experimental procedure carried out by R. Makwana et al. at BARC-TIFR Pelletron facility in Mumbai [2]. Previous studies suggest that a competition will always occur between n and p-emission and in systems where binding energy of neutron is larger, low energy protons are emitted [3]. In this paper, the p-emission cross-sections are addressed via collective clusterization approach of DCM by optimizing the neck-length parameter and DCM based calculations seem to agree with the experimentally available data spanning energies from Ec.m.~17 MeV. The centrifugal energy is an integral part of the total interaction potential occurring between two interacting/outgoing fragments and its influence on the fragmentation patterns is investigated in this work. For this purpose, the sticking and non-sticking limits of moment of inertia are employed the effect on the decay structure is investigated. Since DCM is based on collective clusterization approach which suggests that one exit channel is preformed at the expense of all the possible exit channels emerging from a hot and rotating compound nucleus.

C2- 0011

Study of 12C (p, γ) 13N reaction at astrophysical region

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Abstract

The 12C(p,γ)13N is the first reaction in the Carbon-Nitrogen-Oxygen (CNO) cycle which dominates the energy production in stars with masses heavier than 1.5 $M\odot$ and the12C(p,γ)13N(β+)13C reactions can influence the 12C/13C ratio which is thought to be an important measure for stellar evolution and nucleosynthesis. Using Asymptotic normalization coefficient (ANC) value of ground state of 13N which is taken from Z.H. Li et al. (2010), the astrophysical S-factor and rate of the 12C(p,γ)13N reaction are calculated at astrophysical energies by R-matrix code AZURE2. The value of astrophysical S-factor at 25.0 keV is 1.33 keV b and the rate of this reaction at 0.1 GK is 2.14 x 10-5 cm3s-1mol-1. The current evaluated values are good agreement with the literature values.

C2- 0012

The rate calculation of the astrophysical reaction 12C (α, γ)16O at stellar region

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Abstract

The most two important thermonuclear reactions by which He is decreased are the 3α→ 12C and 12C (α, γ)16O reactions in the He-burning stars. At the end of the He-burning phase, the rate of the 3α→12C and 12C (α, γ)16O reactions determines the 12C/16O abundance ratio, the subsequence nucleosynthesis in massive stars and final fate of the stars. The rate of the strophysical 12C (α, γ)16O reaction is calculated using the astrophysical S-factors and the symptotic Normalization Coefficient (ANC) values of the dominant states 6.92 (2+) and 7.12(1-) eV of 16O at the stellar region (Temperature T= 0.06-10 GK). The astrophysical S-factors and the ANC values of the 6.92 and 7.12 MeV states of 16O are taken from Ashok Kumar Mondal et.al. (2021). the rate of this reaction at 0.06 GK is 7.2 x 10-26 cm3s-1mol-1. The calculated rates in the temperature range 0.06 GK to 10 GK are good agreement with the literature values.

C2- 0013

Determination of astrophysical S-factor and rate of the 14N(p,)15O reaction at stellar region

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Abstract

The 14N(p,γ)15O(Q = 7297 keV) is the slowest reaction in the hydrogen burning CNO cycle.This reaction play vital role in controlling the reaction rate of the carbon-nitrogen-oxygen (CNO) cycle, which is the secondary mechanism for converting hydrogen into helium.we have calculate the S-factor and reaction rate using the *R*-matrix calculation by Azure-2 Code.The astrophysical S-factor value has been measured at the low-energy E=0(Mev) data of Schröder et al.The Asymptotic Normalization Coefficient (ANC) value is deduced from transfer reaction 14N(3He,d)15O for the ground state 15O ANC=4.2fm-1/2 and for excited state(6.79) ANC=0.714fm-1/2 taken from Bertone2002_ANC.The main contribution to the *S*-factor at zero energy comes from transitions state at *Ex*=6.79 MeV (*E*cm = −0.504 MeV),S(0)=0.0761(kev-b) for 6.79(mev), subthreshold state S(6.79)=1.4953(kev-b) and Stot=1.517(kev-b) and rate of this reaction at 0.008GK is 6.07*10^-25 cm3s-1mol-1.The current evaluated values align well with those found in the literature.

D1- 0001

Shape Memory Effect and Crystallographic Aspects of Reversibility in Shape Memory Alloys

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Abstract

Shape memory alloys take place in a class of advanced smart materials, by exhibiting a peculiar property, called shape memory effect, which is characterized by the recoverability of two certain shapes of material at different conditions. Shape memory effect is initiated on cooling and deformation processes and performed thermally on heating and cooling, with which shape of materials cycles between original and deformed shapes in reversible way in bulk level. Therefore, this behavior can be called thermal memory or thermoelasticity.

Thermoelasticity is governed by crystallographic transformations, thermal and stress induced martensitic transformations. Thermal induced martensitic transformation occurs on cooling, with cooperative movement of atoms in <110 > -type directions on the {110}-type plane of austenite matrix, along with lattice twinning and ordered parent phase structures turn into twinned martensite structures by means of lattice invariant shears. The twinned structures turn into detwinned martensitic structures with deformation by means of stress induced transformation. These alloys exhibit another property called superelasticity, which is performed with stressing and releasing the material in elasticity limit at a constant temperature in the parent phase region, and shape recovery occurs instantly upon releasing by exhibiting elastic material behavior. Superelasticity is also governed by stress induced martensitic transformation and ordered parent phase structures turn into detwinned martensite structures with stressing in the parent phase region. Copper based alloys exhibit this property in metastable β-phase region, which has bcc-based structures. Lattice invariant shear and twinning is not uniform in these alloys and gives rise to the formation of complex layered structures. These structures can be described by different unit cells 9R or 18R depending on the stacking sequences on the close-packed planes of the ordered lattice. In the present contribution, and x-ray and electron diffraction studies performed on two copper- based CuZnAl and CuAlMn alloys. Electron diffraction patterns and x-ray diffraction profiles exhibit super lattice reflections in martensitic condition. Specimens of these alloys aged at room temperature in martensitic condition, and a series of x-ray diffractions were taken duration aging at room temperature. Reached results show that diffraction angles and peak intensities change with aging time at room temperature. and this result leads to the rearrangement of atoms in diffusive manner.

D1- 0002

Hydrogen Pipeline and Non-Destructive Methods

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Abstract

The growing demand for hydrogen highlights the need for efficient transportation. Hydrogen pipelines are a cost-effective solution, but they face challenges such as corrosion. Limited research exists on how to choose inspection techniques for maintaining pipeline integrity, especially when long distance supplies are involved. The continuous supply of gas transport pipelines inevitably leads to deterioration in the physical and mechanical characteristics of the pipeline steel, significantly impacting their operational capabilities. This crucial aspect is frequently overlooked during the initial design phase. However, assessing the extent of steel degradation is absolutely essential when evaluating the pipeline's remaining service life. Therefore, it is imperative to thoroughly examine the material deterioration during operation and to utilize non-destructive techniques for assessing steel degradation.This research aims to evaluate the effectiveness of inspection techniques for identifying defects in hydrogen pipelines. We will cover an overview of hydrogen pipelines, common issues, and the use of blended hydrogen-natural gas pipelines. We'll also discuss methods for maintaining pipeline integrity and review-validate current inspection techniques in line with standards such as ASME B31.12 and BS 7910. Lastly, we'll summarize the latest inspection techniques and areas for future research.

D1- 0003

Structural and Optical Properties of $AlAs_xSb_{1-x}$

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Abstract

We present a theoretical investigation of the structural and optical properties of $AlAs_xSb_{1-x}$ semiconducting alloys in zinc-blende structure based on the empirical pseudopotential method within the virtual crystal approximation combined with the Harrison bond-orbital model. The Elastic Constant, bulk modulus, refractive index, high frequency dielectric constant, static dielectric constants are calculated for $AlAs_xSb_{1-x}$. Our results for $AlAsxSb1_{-x}$ ($0<x<1$) are predictions.

D1- 0004

Giant magnetocaloric responses in $Ni_{45}Mn_{43.3}Cr_{0.7}Sn_{11}$ Ferromagnetic Huesler alloy near room temperature for magnetic refrigeration applications

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Abstract

Magnetic-shape-memory-alloys are a unique category of functional materials exhibiting multifunctional properties. Here we investigate the structural, microstructural, magnetic, magnetocaloric (MCE) properties and thermal path dependency of an off-stoichiometric $Ni_{45}Mn_{43.3}Cr_{0.7}Sn_{11}$ alloy in details. The alloy crystallizes in the $L2_1$ cubic austenite-phase having space group Fm-3m and the $L1_o$ tetragonal martensite phase, as secondary, at room temperature(RT). Magnetic studies provide evidence of low coercivity, and Differential-Scanning-Calorimetry and temperature-dependent electrical resistivity measurements verify magneto-structural transition. The investigation of spin fluctuations' impact on magnetic characteristics discloses the existence of long-range weak-itinerant-ferromagnetism. The highest magnetic-entropy-change(ΔS_m) obtained around the FOMT (first-order magneto-structural phase transition) and SOMT (second-order magnetic phase transition) are + 69.16 $J.kg^{-1}K^{-1}$ and - 5.05 $J.kg^{-1}K^{-1}$, respectively, while, a 'working-temperature-span'(ΔT_{FWHM}) of 3.42 K and 3.54 K are found, respectively, under a magnetic field change of 6 Tesla. In the same field, this offers a refrigerant capacity of 173.75 $J.kg^{-1}$ and 17.07 $J.kg^{-1}$; relative cooling power of 236.53 $J.kg^{-1}$ and 17.88 $J.kg^{-1}$ around FOMT and SOMT, respectively, demonstrating that both hold high significance from MCE perspective as well as for refrigeration applications. More importantly, the highest adiabatic-temperature-change(ΔT_{ad}) across FOMT at 276 K at 6 T is found to be -7.62 K. Our investigation shows that, apart from the Arrott plot, the field dependence of the M^3 plot and the exponent n are equally crucial in determination of transition-order and its switching behaviour. All of these MCE characteristics render this alloy a highly promising contender for future use in the field of solid-state magnetic-refrigeration near RT.

D1- 0005

Optimization of Substrate temperature and film thickness in current transport characteristics of SnSe thin film

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Abstract

The behaviour of SnSe thin films depends on the methods used for their preparation, deposition conditions, substrate temperatures and thickness of films in controlling their properties for suitable electronic device applications. Present investigation showed the effect of substrate temperature (550K, 575K and 600K on 200nm thick SnSe films) and thickness (150nm, 200nm, 250nm and 500nm at substrate temperature 575K). The films displayed better crystallinity as well as improved material parameters in order to optimized current transport behavior of the deposited SnSe thin films. The XRD spectra and the SEM analysis suggest that the polycrystalline thin films of SnSe possess orthorhombic structure having uniform distribution of grains along the (111) diffraction planes. It was observed that the crystalline quality, electrical and optical behaviour of the films changed with the film thickness. The analysis of the data obtained from the optical transmission spectra suggests that the films possess energy bandgap in the range of 1.38 - 1.18 eV while resistivity of films falls in the range 112-20 Ω-cm. The analysis of the optical transmission spectra suggests that the bandgap of films deceases (from 1.71 to 1.13 eV) with increase in film thickness (150 - 500nm). A close examination of the investigations reveals that the absorption coefficient (α) decreases with increase in thickness in the high energy region of the plot. The results, thus obtained were found to be better than those of the studies made at room temperature for its current transport behavior and subsequent use in solar cell as absorber layer.

D1- 0006

Annealing effect on Mg-doped NiO nanocrystal prepared by ball milling method

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Abstract

A detailed study of the mechanochemical (MC) processing of milled and annealed Mg-doped x = 5-50 at % powders was carried out using a high-energy ball milling technique to investigate the formation of a NiO-based nanocomposite as a function of the milling time. During milling, the reduction of NiO to Ni follows a gradual process with a reduction in size and a self-sustaining process with a maximum reduction of 94% for $x=50$ powders with formation of nanocomposite of NiO-Ni-MgO. NiO reduction and phase transformation types are studied in detail in milled and annealed samples. The process of time-dependent MC reduction and the resulting structural, vibrational, magnetic, and optical behaviour of the as-milled and insitu annealed nanocomposite were studied in detail. This process may reveal potential applications in metallurgy and ore reduction processes.

D1- 0007

Tribological Aspects And Behaviour of Magnesium Metal Matrix Nanocomposites: An Overview

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Abstract

One of the most fundamental objectives of developing metal matrix composites is to enhance the wear resistance of soft and light weight metals. The addition of nano scale reinforcements in metals has been found to improve the wear losses as compared to their pure counterparts. Being light weight and having widespread application in sports, automobile and aviation sectors, the tribological studies of the magnesium based nano components is under scanner recently. Wear performance of machines with sliding/moving parts is of paramount importance for enhancing life of parts and improving efficiency. Thus Mg based nano components(Mg-MNCS) developed by incorporating nano materials viz. Silicon Carbide (SiC) graphene nano platelets (GNP), Carbon nano tubes (CNT), Titanium Di-boride (TiB_2) and Tungsten Carbide (WC) etc. has been developed to address wear issues. The characteristic of such composites depends on the quantity and nature of the additives besides the fabrication process involved in developing these. In present review implications of different parameters viz. load, sliding speed, reinforcement dose & nature and ambient temperature on tribological behaviour, coefficient of friction (COF), and wear of Mg-MNCs is being examined. Besides this the impact of various fabrication techniques like stir casting (SC), ultrasonic treatment casting (UST) and others on wear and friction behaviour of Mg-MNCs is also looked into.

Keywords: Magnesium nanocomposite, tribological studies, wear resistance, COF, stir casting, wear mechanism.

D2- 0001

Spectroscopic and Computational Insights into Hydrogen Bonding in (S)-(+)-4-Amino-3-hydroxybutyric acid Dimer

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Abstract

In antiepileptic and hypotensive medicines, (S)-(+)-4-amino-3-hydroxybutyric acid is a well-known neuromodulator. From its experimental infrared spectrum, it is evident from the vibrational bands around 3500 cm-1 - 1577 cm-1 that the molecule is an inter-molecular O−H···O/N−H···O hydrogen bonded zwitterion. In this study, molecular dynamical modelling of (S)-(+)-4-Amino-3-hydroxybutyric acid in a solvent yielded several O−H···O/N−H···O bonded dimers and higher oligomer species at production run for 100 ns. The results of the computed radial distribution function indicate that the H···O distances for both types of H-bonds are smaller than the sum of the van der Waals radii of the H and O atoms, 2.72 Å. This supports the two H-bonds existence. Using an implicit SCRF water solvation model, the dimer with the highest Boltzmann population optimized at the B3LYP/6-311++G(d,p) level of DFT exhibited bifurcated inter- O−H···O/N−H··O and N−H···O bonds, supporting the observed IR, VCD, and Raman band characteristics. The experimental ECD spectrum is in good agreement with the computed dimer spectrum at the CAM-B3LYP/6-311G(d,p) level of TD-DFT. The natural bond orbitals, n(O)→σ*(N−H/O-H), with high values of stabilization energies ranging from 8 to 15 kcal/mol indicate the strong hydrogen bonds. The quantum theory of atoms in molecules and non-covalent interactions analyses of electron densities, also support the strong hydrogen bonding in (S)-(+)-4-Amino-3-hydroxybutyric acid dimer.

D2- 0002

Betamethasone: FTIR measurements at temperatures lower than RT

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Abstract

Betamethasone (BM) is characterized by FTIR spectroscopy in KBr pellet at temperatures ranging between RT (300 K) and 103 K, for the first time. Very clear spectral changes are observed in the characteristic stretching regions 2700-3700 cm^{-1} and 1550-1750 cm^{-1}, upon temperature variation. Observed data is compared with the computed data obtained at DFT(B3LYP)/6-311++G(d,p) level of theory. Tentative assignments are provided for some selected observed peaks based on the comparison between experiments and the theory. A possible phase transition is suggested to occur at low temperatures below 280 K.

D2- 0003

Electron emission from H_2O molecule by the impact of 600 keV bare helium ions

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Abstract

Water is an essential part of biological systems, knowing how it reacts to ionizing radiation is important for applications in radiation therapy, where precise energy deposition modeling is essential for both treatment efficacy and patient safety [1, 2]. Furthermore, by offering experimental benchmarks for theoretical models like the Continuum-Distorted-Wave Eikonal-Initial-State (CDW-EIS) model, which are used to forecast the results of ionizing events in more complex systems, the collected data benefit the larger field of atomic and molecular physics [3]. This information is crucial for expanding our overall understanding of how radiation interacts with materials as well as for enhancing medical applications. The significance of this study lies in its contribution to our comprehension of ion-molecule interactions, particularly the kinetics of ionization of water molecules under the influence of high-energy helium ions.

This work reports on an electron spectroscopy study carried out at the Tata Institute of Fundamental Research (TIFR), Mumbai, India, on water molecules ionized by 600 keV bare helium ions. A high-resolution electron spectrometer was used for the experiment, measuring the double-differential cross sections (DDCS) of electrons emitted over an energy range of 1–600 eV and scattering angles ranging from 20° to 160°. The experimental data were compared with theoretical predictions based on the Continuum-Distorted-Wave Eikonal-Initial-State (CDW-EIS) model in both prior and post forms. The results show a good overall agreement with the CDW-EIS model, with the prior version providing a better match for the angular distributions at forward angles.

D2- 0004

Information theory of 2-electrons in a circular box: Effect of confinement and external perturbation

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Abstract

Two particle systems is explored in the context of information theory. This kind of system is interesting owing to its application, not only in the information theory, but in many related areas. The interaction between the particles plays a very important role in determining the outcome. The interaction can be explored in three different regions. **(a)** Strong confinement region: where confinement is dominant over the interaction between the particles. **(b)** The moderate confinement region: where confinement and interaction between the particles compete with each other to affect the outcome. **(c)** The weak confinement region: where interaction between electrons dominates the outcome.
The work is divided in two parts. **(i)** The information measures of the system are calculated without external perturbation, **(ii)** The effect of external perturbation, for example, static electric field, magnetic field and weak laser fields on the information theory of the system. The effect of external perturbation parameters on information theory measures are explored in detail.
With the application of confinement, the energy and information theory measures of the system under consideration can be modified [1-4]. For weak confinement the interaction energy is dominant. For moderate range, the interaction energy becomes comparable to the energy due to confinement. For strong confinement region the energy due to confinement is large enough and the interaction energy loses its significance [4]. Also, the external perturbation applied on the system, modifies the dynamics resulting in modifying the energy and information theory measures [3,5-7].

D2- 0005

Theoretical Studies of Electron Impact cross sections for the Atomic Targets Mg and Ca

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Abstract

The electron impact ionization on the Martian dust is occurring on mars. In this paper, we have calculated electron impact ionization cross-sections of Magnesium and Calcium in the energy range of 10 - 2000 eV. Mg and Ca are present in the martian atmosphere in trace amounts, in the form of ions. Mg can provide insights into Martian dust and surface materials.
Spherical Complex Optical Potential (SCOP) is used to derive the total cross section and determine the inelastic cross section. We use variant Complex Scattering Potential - ionization contribution *v*CSP-*ic* method to calculate ionization cross-sections. Our results are compared with the available experimental and theoretical data.

D2- 0006

Solution and Momentum Spectrum of the Modified Yukawa-Kratzer Potential model

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Abstract

In this work, we calculate the momentum spectrum of the modified Yukawa-Kratzer Potential (MYKP) model using the Supersymmetric quantum mechanics (SUSY) method as applied to different diatomic molecules. We obtained the momentum energy spectrum by solving an associated Riccati equation using partner potentials. Our potential reduces to Screened Coulomb plus modified Yukawa, Kratzer, Modified Yukawa, Hellmann potential, and Coulomb potential as special cases. We obtained momentum eigenvalue spectrum for special cases and compare our work with existing literature. our results for special cases agree excellently for all quantum states using different screening parameters. Also, using the Parametric Nikiforov-Uvarov method, we obtained a total normalized wave function expressed in terms of Jacobi polynomial. With the help of well-designed Mathematica programming, we obtained wave function and probability density plots for four diatomic molecules for fixed orbital angular quantum numbers l = 0, 1, and 2 with varying quantum states n = 0, 1, 2, and 3. The current research has applications in physical and chemical physics and molecular spectroscopy.

D2- 0007

Construction of an artificial molecule using molecular modelling software aided by atomic & molecular physics in math model

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Abstract

The project titled "*Construction of an Artificial Molecule Using Molecular Modelling Software Aided by Atomic & Molecular Physics*" focuses on the design and simulation of an artificial molecule through advanced computational techniques. Leveraging molecular modeling software, the project integrates principles from atomic and molecular physics to construct and analyze a molecule with custom properties. The modeling process involves the precise calculation of atomic interactions, bond formations, and electron distributions to achieve desired molecular structures and functionalities. By simulating quantum mechanical behaviors and optimizing molecular geometry, this research aims to create a highly stable and functional artificial molecule. The use of atomic and molecular physics ensures that the interactions at the quantum level are accurately represented, facilitating the exploration of novel molecular configurations that may have potential applications in materials science, drug design, and nanotechnology. This project demonstrates the power of molecular modeling software in advancing the field of molecular engineering, providing a framework for designing artificial molecules with specific, targeted properties. Molecular modelling covers a wide variety of theoretical and computational methods used to represent the structure of molecules, ions and/or particles. They can be classified—according to the length and time scale of the modelling matter—from electronic to continuous levels. Considering solute/solvent systems, there are three main categories for molecular modelling: implicit methods, integral equations and classical density functional theory, and explicit methods. Thus, in order to present the main idea of each class of methods available in chemical engineering field, this work comprehends three methods: Poisson Boltzmann equation, classical density functional theory, and molecular dynamics simulation. Finally, scale integration is presented as a strategy for efficient modelling and simulation.

E1- 0001

Exploring the conformational changes in the crystal structure of human telomeric DNA G-quadruplex with ligand/inhibitors caffeine derivative through docking

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Abstract

G-quadruplex are formed near the telomeric region of chromosomes for the sequences having multiple of Guanines nucleotide. Plenty of guanines associated together to build quadruplex secondary structure based on non-Watson-Crick base pair model. We perform computational methods to study the G4 structure-ligand interactions which may generate informations that cannot be accessed experimentally. We report here the conformational changes in quadruplex structure and binding affinity of ligand caffeine derivatives. The co-ordinates of human telomeric DNA G-quadruplex were retrieved from the database with PDB ID 6XCL. Screening of the 10 caffeine derivative ligands have been performed through docking within the binding site of the quadruplex. Out of all Ligands some show better binding capabilities than the ligand **Platinum(II)-bis[3-(pyridin-2-yl)-[1,2,4]triazolo[4,3-a]pyridine]** bound within the crystal structure, as have been concluded on the basis of docking scores and noncovalent interactions.

E1- 0002

Dielectric Spectroscopy for Drug-Amino Acid Characterization

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Abstract

Dielectric Relaxation Spectroscopy (DRS) gives the dielectric response from the materials under study at different concentrations and temperatures using time domain reflectometry technique in the frequency region 1 GHz to 50 GHz. Dielectric parameters for the non-steroidal anti-inflammatory drug (NSAID) aceclofenac, diclofenac, in aqueous solutions of amino acids Valine and Leucine can be explored in terms of complex permittivity (ε*), dielectric constant (ε), dielectric relaxation time (τ), dipole moment (μ) and Kirkwood correlation factor (g). Displacement of the charges in the material under test exposed to microwave radiation gives polarization and the energy required for the dipoles to be polarized can be interpreted in terms of thermodynamic parameters such as enthalpy of activation (ΔH), entropy of activation (ΔS) and free energy of activation (ΔF) to give more insight into the structural dynamics of the materials. The structural information gives specific properties of the material and ultimately useful to target applications.

Keywords: Time Domain Reflectometry; Dielectric Relaxation; Drug; Amino acid; Thermodynamic Parameter.

E1- 0003

Microscopic analysis of calcium phosphate (CaP)/ Poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV)polymer Composites

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Abstract

In this present contribution Calcium phosphate (CaP)/ Poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV)polymer nanocomposites have been fabricated via solution casting method and characterized. These composites are biocompatible in nature so that they used in bone tissue application. CaP has filler or nanofiller of polymer matrix composite. CaP filled polymer matrices are used for fabricate substrate and also used bone regeneration scaffolds. CaP has been dispersed into PHBV polymer into weight ratio 1 to 5%. The X-ray diffraction spectra confirm crystalline phases in CaP/PHBV composites. FT-IR spectra confirm bonding orientation between CaP and PHBV polymer. The SEM images showing homogeneous dispersion of CaP into polymer composites.

E1- 0004

Invitro Therapeutic Activities of Copper Oxide Nanoparticles Impregnated Biocidal Film by Phyto Induced Reduction Method

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Abstract

The wound healing process is very important since it is essential to regaining the integrity and function of broken tissues or organs. One of the primary challenges for wound healing during the pandemic has been delays in seeking medical care from hospitals due to concern about virus exposure. Copper is one of the bioactive nanoparticles that plays a complex role in a variety of cells. It alters the mechanisms of action of numerous cytokines and growth factors, and it essentially contributes in every stage of the healing process for wounds . In this study, Ixora coccinea leaf extract was employed as a reducing agent to create Cu nanoparticles in a sustainable manner. Ancient Indian traditional systems used the plant Ixora coccinea for its therapeutic properties. Several flavonoids and alkaloids found in the leaf extract are known to possess antibacterial actions against a wide range of bacterial strains. Taking advantage of UV-visible spectroscopy, FTIR, and SEM to analyse the synthesised Cu nanoparticles, it was found that they were stable. Likewise a polyvinyl alcohol (PVA) matrix was made using the synthesized Cu nanoparticles and glutaraldehyde as a cross-linking agent. The PVA-Cu NPs film that was generated will evaluate stability, swelling behaviour, antibacterial activity, and in vitro effectiveness. Findings explain that the PVA-CuNPs film had strong antibacterial action against Staphylococcus aureus and Escherichia coli, good stability and negligible swelling behaviour in phosphate-buffered saline (PBS). These results show the PVA-CuNPs film's potential as a promising wound healing material that may successfully fight bacterial infections and encourage tissue regeneration. Future applications will be very important for the green synthesis method, as it provides a sustainable and environmentally friendly alternative to traditional synthesis techniques that rely on harmful chemicals and produce hazardous waste. The PVA-CuNPs film developed in this work has the potential to transform wound healing and open up possibilities for the creation of more long-lasting and efficient wound healing materials.

E1- 0005

Silkbot - Orchestrating Silk Symphony - A comprehensive Approach Towards Silk Production and Enhancement using silk nano materials

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Abstract

The project titled "Silkbot - Orchestrating Silk Symphony: A Comprehensive Approach towards Silk Production and Enhancement Using Silk Nano Materials" aims to revolutionize the silk industry by integrating cutting-edge technology with traditional silk production methods. By developing an automated Silkbot system, this project seeks to address critical challenges in the silk production process, from cocoon segregation to optimizing environmental conditions for silkworm growth. This initiative envisions enhancing the quality and quantity of silk output while reducing wastage and disease spread, thus contributing to more sustainable and efficient silk farming practices. Silk production, an age-old industry, is deeply rooted in various regions of the world and plays a significant role in economic growth, especially in countries like India and China. Despite advancements in sericulture, many challenges still hinder optimal silk production, including improper cocoon segregation, widespread diseases, and suboptimal growth conditions for silkworms. The "Silkbot" project aims to overcome these obstacles by employing advanced automated systems that provide a comprehensive, technology-driven solution for silk producers. This project integrates gender-based cocoon segregation, diseased cocoon identification, temperature control, and feeding optimization to improve the overall silk production process and enhance the quality of the silk produced.

E1-0006

Algae-Based Biomolecules for a Sustainable Future in India: Opportunities and Challenges

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Abstract

Over the past decade, algae have emerged as pivotal organisms, increasingly acknowledged for their profound ecological contributions and cutting-edge technological applications, particularly in the development of eco-friendly biomolecules. India's tropical climate and abundant sunlight create ideal conditions for large-scale algae cultivation, with oceans rich in microalgae, diatoms, and dinoflagellates. Of the 30,000 to 40,000 species, only a few are commercially utilized, but more can be explored for environmental, energy, and food security benefits. This review investigates algae-derived natural, carbon neutral biomolecules production and highlighting its scope and challenged in India It also outlines how algae can drive sustainability across sectors such as bio plastics, biofuels, food, cosmetics, and pharmaceuticals, along with emerging trends in the fashion industry like biobeads and bioleather. By lowering costs and reducing carbon emissions in algal biorefineries, these strategies contribute to a sustainable future. However, obstacles such as the energy-intensive production process and the need for optimized biorefinery pathways impede large-scale commercialization. Moreover, India's algae products market faces challenges, including low consumer awareness, difficulties in ensuring sustainable sourcing, and strict regulatory standards. Competition from conventional products, coupled with the need for continuous innovation to improve taste and versatility, further complicates market expansion.

E1-0007

Investigation of Linear and Nonlinear Optical Properties of Natural dyes

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Abstract

Nonlinear optical (NLO) materials play a vital role in the development of future technologies and industrial applications. However, advancements in this field have been constrained by the limited availability of materials that meet the necessary optical and environmental criteria. This has led to extensive research focused on creating enhanced NLO materials. A significant development has been the discovery of third-order optical nonlinearity in natural materials, which holds great potential for use in photonics and optoelectronics. In this study, natural dyes were obtained from Ixora coccinea and red sandalwood using a cold extraction process . The third-order NLO characteristics of these dyes were investigated using the single-beam Z-scan technique with nanosecond laser pulses at a wavelength of 532 nm. The results suggest that these natural dyes show strong potential for application in the development of photonic devices.

E2- 0001

Hall Effects on MHD Convective Flow through Porous Medium past an Infinite Vertical Plate with Soret Effect and Dissipation

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Abstract

We have studied the combined effects of MHD mixed convective two dimensional flows of an incompressible and electrically conducting viscous fluid through porous medium past an infinite vertical plate taking Soret, Joules dissipations and Hall effects into account. The non-dimensional equations are then solved analytically using perturbation technique. With the help of graphs, the effects of the various non-dimensional parameters on velocity, temperature and concentration distributions within the boundary layer are examined. Also the effects of the pertinent parameters on the skin-friction coefficient and rates of heat and mass transfer in terms of the Nusselt and Sherwood numbers are computationally discussed.

Keywords - Hall effects, Heat source; Soret number; Porous medium; Joules dissipation; MHD; Chemical reaction.

E2- 0002

Motion of Strong Detonation Waves in Rotating Real Gas

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Abstract

The behavior of real gas behind the strong detonation wave's front is analyzed with the help of Chester-Chisnell-Whitham (CCW) theory. The medium is supposed to be reacting real gas including the solid body rotation. The density of the gas ahead of the imploding detonation front is assumed to be power varying. It is assumed that detonation wave is initially Chapman-Jouguet. The expressions for the detonation velocity and other flow variables are derived. Neglecting the effect of Coriolis forces, the effect of solid body rotation of reacting gas on detonation velocity and other flow variables has been estimated. The variation of detonation velocity, non-dimensional pressure and non-dimensional flow velocity with convergence of detonation front, density parameter, specific heat ratio of gas have been discussed though graphs in details. Finally, it is observed that density parameter, adiabatic index and Alfven Mach number of gas have significant effect on all the flow variables.

E2- 0003

Role of Interaction on The Performance of A Coupled Diffusion Brownian Motor

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Abstract

In recent years, noise, usually seen as a hindrance, has been found to have many constructive aspects as well. One area in which noise is seen to play a beneficial role is that of Brownian motors: nano-scale or micro-scale devices which rectify thermal fluctuations in presence of broken symmetry when driven out of equilibrium. While many investigations have been carried out on Brownian motors composed of a single Brownian particle there are comparatively fewer studies regarding the role of interaction between Brownian particles on the performance of the motor. In this work we investigate how coupling between Brownian particles affects the performance of a Brownian motor driven by time-dependent temperature heat bath. We find there exist optimal values of various parameters such as the temperature, coupling constant, number of Brownian particles, asymmetry of the substrate potential at which the performance of the motor reaches a peak.

F1- 0001

The fabrication and characterization of Zinc Phosphate

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Abstract

Zinc acetate was treated with phosphoric acid and by using the chemical precipitation method, zinc phosphate particles were obtained. Without using chemical hydrazine, the approach aims to synthesize zinc phosphate in the simplest possible way in terms of particle dimensions. To identify the synthesized substance and reveal the information or materials for which it is designed, several characterization procedures were employed. X-ray Diffraction, Ultraviolet-Visible, Scanning Electron Microscopy, Raman Spectroscopy and Fourier Transform Infrared were utilized to analyze the synthesized particle. The FTIR spectra are used to analyze the stretching and bending frequencies of the molecular functional groups in the material. When using XRD, the morphology of the zinc phosphate particles was identified. The obtained product Zinc (II) Phosphate has well-crystallized particles, as seen in the SEM image. The UV spectrum notifies the different electronic excitation states of Zinc (II) Phosphate. The peaks of the Raman spectra confirm the presence of zinc phosphate, which was prepared using zinc acetate and phosphoric acid in a relatively simple manner.

F1- 0002

Experimental Research on The Efficiency of Photovoltaic Cells for The Conversion and Storage of Solar Energy

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Abstract

The conversion and storage of solar energy was investigated utilizing the Rose Bengal - Oxalic acid - Cetryl hexadecyl ammonium bromide System in conjunction with the photogalvanic effect and photo galvanic cell. In an aqueous solution, cetryl hexadecyl ammonium bromide serves as a charge transfer carrier, raised Bengal as a sensitized dye, and oxalic acid as a reductant. 550.0 mV of photo potential and 75.0 µA of photocurrent were produced, respectively. At its power point, the cell's observed power was 41. 3 µW. The results showed that the fill factor and conversion efficiency were, respectively, 0.169 and 0.067%. In the dark, the cell performed for 175.0 minutes. Additionally, a photogeneration technique for electricity production has been proposed. The impact of several factors on the electrical output of the cell was studied by plotting a curve between current and voltage.

F1- 0003

Synthesis and Characterization of Zero Valent Iron Nanoparticles

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Abstract

In the present work, nano zero valent iron (nZVI) were synthesized by the method of hydrated ferrous sulphate (FeSO4.7H2O) reduction using sodium borohydride (NaBH4) as a reducing agent under ambient conditions. Characterization of nZVI was performed using XRD and FTIR. The acquired iron nanoparticles are mainly in zero valent oxidation state. The obtained results were close agreement with other experimental works.

F2- 0002

Fractal Geometry, the Da Vinci of Mathematical Science

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Abstract

This paper presents a unique collection of fractal designs that simulate a diverse range of natural and man-made phenomena, from African and Indian masks to human body, face, and even bacterium structures. Paper demonstrates how these fractal designs can be used as a modern art form, transforming spaces such as homes, offices, and hospitals into calming environments. The intricate patterns and self-similarities of fractals have been shown to have a therapeutic effect, reducing anxiety, depression, and mental fatigue. Some fractal art pieces, inspired by Kundalini and Mandala arts, offer a unique blend of mathematical beauty and cultural significance. By integrating these fractal designs into modern spaces, author provides an innovative solution for promoting mental well-being and serenity. This interdisciplinary work bridges the gap between mathematics, art, and therapy, opening new avenues for the application of fractal geometry in enhancing human experience.

F2- 0002

Applications of Newly Discovered Orthogonal Polynomials in Quantum Theory

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Abstract

In quantum theory, the solutions of most of the solvable systems are related to the well-known classical orthogonal polynomials namely the Hermite orthogonal polynomials, Laguerre orthogonal polynomials or the Jacobi orthogonal polynomials etc. In this work, listed all the newly discovered orthogonal polynomials (also known as exceptional orthogonal polynomials) with their important properties and discuss their applications in searching of new solvable systems. We further show that the solutions of these solvable potentials can also be written explicitly in terms these exceptional orthogonal polynomials.

Keywords: Solvable system; Classical orthogonal polynomial; Exceptional orthogonal polynomial.

G1- 0001

Effect of Bismuth doping in surface and mechanical properties of Barium

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Abstract

In the present work the effect of different concentrations of bismuth substitution in barium titanate shall be explored. Bismuth doped Barium Titanate (Bi-doped BaTiO3) ceramics exhibit interesting mechanical and surface properties due to the incorporation of bismuth ions into the BaTiO3 crystal lattice. Bi-doped BaTiO3 ceramics typically show enhanced dielectric properties compared to pure BaTiO3. This enhancement is due to changes in the crystal structure and the introduction of defects caused by bismuth doping. This paper will relate the dielectric mechanical and surface properties of Bismuth doped Barium Titanate Ceramics. The mechanical strength of Bi-doped BaTiO3 ceramics can be influenced by the doping level and the grain structure. Higher doping levels or specific doping configurations alter the grain boundaries and mechanical behavior, affecting properties like fracture toughness and hardness. This work will present the dependence on the specific bismuth doping concentration, processing methods, and intended applications of these ceramics.

G1- 0002

Influence of Samarium (Sm), Manganese (Mg) and Chromium (Cr) doping on the Multiferroic properties of Bismuth Ferrite.

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Abstract

In this article enhancement in multiferroic properties through Sm doping at Bi site and Magnesium (Mg) and Chromium (Cr) co-doping at Fe site of Bismuth Ferrite has been reported. All samples of $Bi_{0.88}Sm_{0.12}Fe_{0.90}Mg_{0.10-x}Cr_x$ for x=0.2, 0.4 and 0.6 were synthesized using Solid State Reaction method. Rietveld refinement on the data obtained through X-Ray Diffraction (XRD) analysis was utilized to identify the phase formation and structural information. Microstructure of all the synthesized samples was studied using Field Emission Scanning Electron Microscopy (FESEM). To verify the dielectric nature of all the samples dielectric analysis was carried out with the help of LCR meter. M-H measurement for all the samples was carried out utilizing the Vibrating Sample Magnetometer (VSM). To investigate the influence of doping on ferroelectric properties of synthesized samples P-E loop was obtained using ferroelectric test system. The effect of Cr doping on enhancing the multiferroic properties of Bismuth Ferrite is discussed in this article.

G1- 0003

Room temperature Multiferroicity in Fe, Zr modified $BaTiO_3$

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Abstract

$BaTiO_3$ (BTO) is a well-known ferroelectric material with tetragonal (*P4mm*) structure. Doping transition metal like Fe in Ti site can impart magnetic ordering in the material and leads to ferromagnetism. However, the incorporation of Fe in Ti site of BTO will lead to paraelectric hexagonal phase (*$P6_3/mmc$*) which deteriorate the ferroelectricity in BTO. To retrieve the tetragonal phase, Zr can be incorporate along with the Fe in Ti site and retains the ferroelectric ordering with incorporation of magnetic ordering in BTO. This will lead to multiferroicity in the material. Multiferroic material $BaTi_{0.94}Fe_{0.03}Zr0_{.03}O_3$ (BZFT) has been prepared through Sol-Gel method. XRD analysis reveals the existence of tetragonal and orthorhombic (Amm2) structure both are ferroelectric in nature. Raman spectrum does not show any peaks corresponding to hexagonal phase and shows tetragonal structure. SEM indicates the well sintered morphology. Temperature dependent dielectric study shows the ferroelectric to paraelectric phase transition at 85 ^{0}C. M-H loop indicate a transition from diamagnetic BTO to antiferromagnetic BZFT with ferroelectric P-E loop. The coexistence of antiferromagnetic ordering with ferroelectric ordering indicates the multiferroicity in this material. The coupling of these ferroic orders can lead to magnetoelectric coupling suitable for various applications in electronic industry.

G1- 0004

Preparation of Tungsten Oxide Doped Borosilicate Glass Adopting Microwave Irradiation for NIR Shielding Application

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Abstract

The cost-effective borosilicate glass was synthesised for NIR-shielding application. NIR shielding energy saving glass system was prepared by adopting microwave (MW) heating method over conventional resistive heating method. The selected chemical composition was $xWO_3 + (15.86 - x)Na_2O + 1.19CaO + 23.81B_2O_3 + 4.37K_2O + 54.4SiO_2 + 0.3TiO_2$ (where x=0 and 1 wt%). The optimized parameters for microwave heating were 2 hr at 1200 °C. The X-ray diffraction (XRD), UV–Vis-NIR and Raman spectroscopy were employed to evaluate the structural and optical properties of tungsten oxide doped borosilicate glass, respectively. X-Ray Photoelectron spectroscopy (XPS) confirmed the chemical state of the tungsten in the glass. The doped borosilicate glass (BSG 1M) was found to have good NIR shielding ability (Tmin ~ 70% at 1050 nm) with acceptable visible light transmittance (Tmax ~ 77% at 550 nm), and hence proposed for applications in NIR-shielding energy-saving windows. The present study emphasizes on tunable NIR-shielding performance of synthesised energy-saving glass. The optimized glass composition can be taken from lab to industrial application and many more endeavors for the manufacturing of energy saving glasses.

Keywords: Near infrared shielding, visible transmittance, Local surface plasmon resonance, Non stochiometric tungsten oxide, Oxygen vacancies

G1- 0005

Study of Structural and Optical Properties of Sm^{3+} doped Lithium tetraborate glasses

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Abstract

This study focuses on optical properties of Sm^{3+} doped different lithium borate glasses. These optical glasses were prepared exploiting the conservative melt-quenching technique. Thermal stability and annealing temperatures were studied for all the glass samples. X-ray diffraction technique is used to examine the amorphous behaviour of glasses. The Fourier Transform Infrared (FTIR) approach enables the observation of the vibrational band locations exhibited by the host material. The chemical composition of these materials has been absolute by the using Energy-Dispersive X-ray Spectroscopy (EDS). Optical absorption were employed in optical research. The evaluation process involves determining various spectroscopic parameters from the absorption spectra, Judd-Ofelt (J-O) parameters (Ω_2, Ω_4, Ω_6), the nephelauxetic parameters (β) along with bonding parameters (δ).

G1- 0006

Structural, ferroelectric and dielectric properties of BaTiO3 and Co-doped Ni-Zn ferrite composites

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Abstract

We report the synthesis and characterization of BaTiO3 (BTO) and Co-Doped Ni-Zn Ferrite i.e.Co0.2Ni0.4Zn0.4Fe2O4 (CoZnNiFeO) composites. BTO and CoZnNiFeO are ferroelectric and ferromagnetic materials, respectively, and these two are used as precursors for synthesizing the BTO-CoZnNiFeO composite. BTO-CoZnNiFeO composites were synthesized using the conventional solid-state reaction method. The samples were sintered at various sintering temperatures ranging from 1000 °C to 1200°C to study the effect of crystallite size on the properties. X-ray diffraction measurements suggest that BTO and CoZnNiFeO possess tetragonal perovskite and cubic spinel structures, respectively, in all the composite samples. The surface morphology and elemental composition of all the samples were examined using field emission scanning electron microscopy. Wide-range X-ray photoelectron spectroscopy survey spectra were obtained for composite samples, revealing peaks corresponding to arious elements like Ba, Ti, Co, Ni, Zn, Fe, and O. Ferroelctric measurements exhibit that the region of the P-E loops increases with the increase of the applied electric field. The losses in P- E loops suggest the low electrical resistive behavior for all the samples. Dielectric measurements indicate the loss remained below one even at high temperatures, suggesting relatively low leakage behavior.

Keywords: Multiferroic, Ferroelectric,X-ray photoelectron spectroscopy, Dielectric

G1- 0007

Flexible Peroxide-Cured Silicone Rubber Composites: Structural, Morphological, and X-ray Detector Performance Analysis

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Abstract

In this study, a soft and flexible polymer composite of silicone rubber was synthesized by incorporating varying concentrations of a peroxide curing agent using the solution casting method, a cost-effective method at room temperature. The synthesized composites were characterized through Energy Dispersive X-ray Analysis (EDAX) and Scanning Electron Microscopy (SEM) to determine elemental composition and surface morphology. SEM micrographs revealed a smooth surface with uniformly distributed crystallites, forming a matrix-like arrangement. Additionally, X-ray switching response measurements were recorded at different voltages to evaluate the detector performance of the composite material. It was observed that detector is showing the photo-response but the difference in photocurrent and dark current needs to be enhanced by adding conducting fillers in the matrix of silicone rubber. The results suggest that peroxide concentration significantly influences the structural, morphological, and detector response properties of the silicone rubber composite, offering valuable insights into optimizing curing conditions for enhanced material performance and detector efficiency.

G1- 0008

Electrical properties of Li2Pb2Dy2W2Ti4V4O30 ferroelectric ceramics

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Abstract

A polycrystalline ceramic, Li2Pb2Dy2W2Ti4V4O30, was synthesized by a traditional mixed-oxide method at a moderate temperature. The material's growth under the specified conditions was previously confirmed using an X-ray diffraction technique. The frequency-dependent change of the dielectric constant might indicate the prevailing polarization within a specific frequency range of the molecule. Analysis of the materials' electrical properties was conducted using the impedance spectroscopy method. Systematic investigation of impedance and its associated factors indicates that the electrical characteristics of the material are significantly influenced by temperature and are well correlated with their microstructure. Electrical phenomena in the material occur as a result of its bulk properties. Accurate determination of the bulk resistance utilizing complex impedance spectra reveals a negative temperature coefficient of resistance. Increasing temperature shifted the peaks in the loss spectrum towards higher frequencies, showing the relaxation process within the system. An analysis of the complex electric modulus indicates that only the grain effect contributes to the total capacitance. The variation of the imaginary part of the electric modulus with frequency is associated with the short-range mobility of charge carriers. There is great interest in studying ferroelectrics of a new class of tungsten-bronze vanadate structure, Li2Pb2Dy2W2Ti4V4O30, as it has found application in microwave devices and electric tunable devices.

G1- 0009

Synthesization of Sr Doped Mn-Zn Ferrite

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Abstract

In the present study, the synthesization of Sr doped Mn-Zn ferrite with the general formula $Mn_{0.6-x}Zn_{0.4}Sr_xFe_2O_4$ was done by using conventional solid state reaction method. Here, the concentration of Sr at Mn cite was of the order of (x=0.0, 0.05, 0.10, 0.15, 0.20) . The raw oxides powdered chemicals were used of Sigma Aldrich (Mn_2O_3, SrO, ZnO, Fe_2O_3) and mixed according to their molar ratio. These powdered chemicals were ground by agate mortar-pestle for 8h. The grained samples were calcined at 900^{o}C and sintered at temperature 1260^{o}C. The samples were characterized using an X-ray diffraction (XRD) for the phase investigation. The Sr^{2+} ions substitute for Mn^{2+} within the ferrite structure, introducing lattice distortion due to the larger ionic radius of Sr^{2+}. X-ray diffraction (XRD) analysis confirmed the formation of a single-phase spinel structure, with an increase in lattice constant corresponding to the Sr^{2+} concentration.

Keywords: Mn-Zn Ferrite, Sample Synthesization and X-ray diffraction (XRD)

G1- 0010

Structure-dependent electrical properties of Ba_2FeNbO_6

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Abstract

There has been significant interest in lead-free ferroelectric ceramics with double perovskite structures due to their lack of toxicity and interesting electrical characteristics. Double perovskites have evolved into an important class of materials and have the potential to be used in various applications such as transistors, capacitors, sensors, etc. due to their versatile properties. In this study, the double perovskite oxide Ba_2FeNbO_6 (BFNO) was synthesized and characterized using X-ray diffraction (XRD), Field Emission Scanning Electron Microscopy (FESEM), and Energy Dispersive X-ray Spectroscopy (EDX). The XRD pattern was analyzed using Rietveld refinement, yielding a cubic structure with cell parameters a = b = c = 8.1165Å, unit cell volume V = 534.7028Å^3, and a calculated density of 6.453 g/cm^3. The reliability factors such as R_p = 11.4%, R_{wp} = 15.5%, R_{exp} = 11.8%, and χ^2 = 1.72 indicate the proper matching of the experimental data with the modeled data. The average grain size was determined from FESEM and found to be 0.754 µm. Impedance and dielectric properties were investigated over a wide range of frequencies and temperatures. The frequency variation dielectric parameters represent the normal behavior of BFNO. The Cole-Cole plot indicates the contribution of grain on the electrical properties of the studied sample. These findings provide insight into the structural and electrical properties of BFNO, contributing to its potential use in advanced electronic and energy storage applications.

Keywords: Double Perovskites, XRD, Complex impedance, Rietveld refinement

G1- 0011

Strong Magneto-dielectric response in $Pb_{0.8}Nd_{0.2}(Zr_{0.52}Ti_{0.48})O_3$ and $SrFe_{12}O_{19}$ based bi-phase composite

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Abstract

Magneto-dielectric composites $(x)Pb_{0.8}Nd_{0.2}(Zr_{0.52}Ti_{0.48})O_3$-$(1-x)SrFe_{12}O_{19}$ with x = 0.5, 0.52, 0.54, 0.56, 0.58 were prepared by solid state reaction method. Structural, microstructural, magnetic, dielectric and magneto-dielectric properties have been explored for all prepared composites. Successful synthesis of bi-phase composites without any impurity phase is established by XRD studies. Microstructural characterization using FESEM reveals uniform and crack free grain growth. Magnetic ordering in all composites with large saturation magnetization (M_s), remanent magnetization (M_r) and coercivity (H_c), is confirmed from M-H hysteresis studies. All composites exhibit large dielectric constant, among which composite with x = 0.54 shows best dielectric response. Dielectric constant value for this sample is 24000 in low frequency (100 Hz) and 1800 in high frequency (1 MHz) range. Magneto-dielectric response (MDR) is observed in all prepared composites. Especially, strong magneto-dielectric effect is seen in composites with x = 0.5 and 0.52 in low frequency region, which significantly extends in high frequency (>100 KHz) region indicating a coupling between electric and magnetic orders in our composites. Coupling coefficient 'γ' is calculated for composite samples (x = 0.5 and 0.52) exhibiting best MD response.

G1- 0012

Multiferroic Properties of PVDF + ($CeFeO_3$-$PbTiO_3$) Composites for Flexible Electronic Applications

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Abstract

Materials with multifunctional properties are important in technological and scientific industries [1]. The importance of flexible electronic materials is increasing for a wide range of advanced technologies including flexible sensors and wearable electronics [2]. This study focused on the multiferroic properties of PVDF+($CeFeO_3$-$PbTiO_3$) composites. The composites aim to utilize the ferroelectric and magnetic properties of CeFeO3-PbTiO3 within the flexible and electroactive polymer polyvinylidene fluoride composites (PVDF) for multifunctional material applications. Traditional materials lack flexibility, so making a material flexible is a priority [3]. The structural, electrical, and magnetic properties of filler content have been studied thoroughly, using different weight percentages of $CeFeO_3$-$PbTiO_3$. X-ray diffraction has been implemented for structural analysis. The microstructural analysis has been performed using a field effect scanning electron microscope (FESEM). Ferroelectric and dielectric properties have been measured using a PE loop tracer and impedance analyzer, respectively. The magnetic properties have been utilized with a vibrating sample magnetometer (VSM). These findings suggest that PVDF + ($CeFeO_3$-$PbTiO_3$)) composites are highly promising for use in energy storage systems, and multifunctional devices where flexibility is crucial. This study contributes to the growing field of polymer-ceramic composites, offering valuable insights into the design of materials with enhanced multiferroic properties for multifunctional applications.

G1- 0013

Structural Characterization, Raman Spectroscopy and FTIR Spectroscopy Studies of Pr^{3+} Doped Tellurium Bismuth Borate Glasses

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Abstract

A series of undoped and Pr^{3+} doped Tellurium Bismuth Borate glasses with composition 20TeO2:(30-X)Bi2O3:50B2O3:(X)Pr2O3 (Where X= 0, 0.1, 0.3, 0.5, 0.7 mol%) have been fabricated via standard melt quenching technique. X-ray diffraction (XRD) patterns revealed that all fabricated glasses were fully amorphous material. The refractive index, density, optical absorption, FTIR and Raman spectroscopy have been applied to investigate the structural and optical properties. FTIR spectral measurements have been utilized to identify the network vibration of Pr2O3 doped Tellurium glasses. FTIR shows B-O stretching (BO3)-units and symmetrical stretching vibration of Te-O in TeO4. Signals in the FTIR mainly observed around 815cm^{-1} - 954cm^{-1}, 1174cm^{-1} - 1180cm^{-1}, 1498cm^{-1} - 1532cm^{-1}, 1765cm^{-1} - 1803cm^{-1} and 2549cm^{-1} - 2672cm^{-1} while Raman scattering peaks are located at 442cm^{-1}, 539cm^{-1}, 767cm^{-1}, 941cm^{-1} and 1024cm^{-1}.

G1- 0014

Synthesis and Spectroscopic Investigations of Rare Earth Pr^{3+} Doped Phosphate Glasses

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Abstract

This paper reports a new series of glass systems (5-x) P_2O_3:40Li_2O:55B_2O_3:xPr_2O_3 (x=0, 0.3, 0.5, and 0.7 mol%) samples prepared using conventional melt-quenching technique. The X-ray diffraction pattern confirms the amorphous nature of the glass system. The refractive index varies from 1.6621 to 1.6641 as the amount of Pr^{3+} increases. The Raman spectroscopy measurement shows that B-O-P bonds were present in the glasses and a Fourier-transformed infrared (FTIR) spectrometer was used to inspect the structural changes of the glasses. From the absorption studies, the value of the optical band gap $E_{opt.}$ has been evaluated. The density parameter, several physical properties, and Urbach energies of Pr^{3+} doped phosphate glasses were calculated. The decrease in optical band gap values and consequently the increase in Urbach's energies confirm the increase in the width of localized states in the band gap.

G1- 0015

Physical, Optical and EPR studies of Magnesium Alumino Borate glasses containing Cu^{2+} ions

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Abstract

In this study, (30-x) MgO-xAl_2O_3-$69.5B_2O_3$-$0.5CuO$ glasses were synthesized using the conventional melt and quench method, and the role of MgO and Al_2O_3 in dictating their physical, optical and EPR studies were investigated. Peak free X-ray diffractograms confirmed the amorphous nature of the glass samples. The decreasing density values of the current glasses suggest structural changes due to the increase in Al_2O_3 content. Al_2O_3 interacts with the glass composition, forming AlO_4 and BO_3 units along with non-bridging oxygens (NBOs). Based on density and molar volume measurements, the oxygen packing density (OPD) and ionic packing densities are calculated. Spectroscopic studies such as optical absorption, EPR were studied to understand the effect of modifier oxide and CuO dopant. From EPR spectra the spin-Hamiltonian parameter were evaluated. The ground state of Cu^{2+} is $d_{x^2-y^2}$ ($^2B_{1g}$ state) and the site symmetry around Cu^{2+} is tetragonally distorted octahedral. A broad optical absorption band was observed for all the glasses containing Cu^{2+} ions corresponding to the $^2B_{1g} \rightarrow {}^2B_{2g}$ transition. The optical band gap and Urbach energy values are calculated.

G1- 0016

Effect of Ge additive on the morphological and physical properties of $Se_{100-x}Ge_x$ (x = 0, 1, 2, 4, 6, 10, 15 and 20) chalcogenide system.

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Abstract

Ge additive chalcogenide materials have become more prevalent in contemporary optoelectronics. The present study utilizes the melt-quenching process for preparing Se-Ge chalcogenide glasses. For the examined system, submicron structural and physical characteristics are examined and described. X-ray diffraction spectra show no characteristic peaks, this indicates that the glassy compositions under investigation are amorphous. A further confirmation of the amorphous nature is provided by SEM. The physical properties of the compositions under examination namely average coordination number (<r>), mean bond energy (<E>), cross linking density (X), lone-pair electrons (L), fraction of floppy modes (f), constraints (N_c), electronegativity (χ), cohesive energy (CE), glass transition temperature (T_g) and heat of atomization (H_s) have been deduced in regard to the influence of Ge content. The mean bond energy has been derived from the chemical bond ordering model, whereas the chemical bond approach (CBA) is utilized for calculating the cohesive energy. The band gap of the investigated system has been calculated theoretically by Shimakawa's relation and the deduced results are analyzed through cohesive energy, electro-negativity and average single bond energy. A correlation has been found between the mean coordination number and various estimated physical parameters.

G1- 0017

Microwave hybrid sintering of $K_{0.47}Na_{0.47}Li_{0.06}NbO_3$ + ZnO ceramics and studies of structural, electrical and piezoelectrical properties

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Abstract

The $Na_{0.47}K_{0.47}Li_{0.06}NbO_3$+(x)ZnO ceramics where x=(0.0, 0.5, 1.0, 1.5, 2.0) wt% were prepared by ceramic route and sintered by microwave hybrid technique. The ceramics were calcined at 850°C for 3h and sintered 1000°C for 20 min. X-ray diffraction (XRD) studied the structural properties and confirmed the formation of tetragonal perovskite phase in all the prepared samples. It is found that crystallite size increased, density improved and hence porosity reduced with addition of ZnO. Scanning electron microscopy revealed the microstructural characteristics development of the niobate ceramics with varying concentration of ZnO. Addition of ZnO in $Na_{0.47}K_{0.47}Li_{0.06}NbO_3$ ceramics and sintered by microwave hybrid technique have shown improvement in grain growth, density, dielectric constant, ac conductivity as well as piezoelectric property. The frequency variation of electrical properties such as dielectric constant, dielectric loss, a. c. conductivity found a dispersive behavior. PE loop traced out of the samples showed ferroelectric behavior with maximum remanance obtained at 1wt% of ZnO addition and piezoelectric properties d33 for this ceramic showed the highest value. The energy storage properties of the prepared samples were systematically investigated and sample with 1 wt% ZnO showed the highest value. The results obtained out of the various investigations have been discussed in the paper.
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Keywords: Sodium potassium niobate (KNN), ZnO, Microwave hybrid sintering, XRD, SEM Electrical properties

G1- 0018

Microwave Dielectric properties of Combustion synthesized $RAlO_3$ (R=Gd, Nd, Sm, Pr and Dy)

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Abstract

The study of superconducting substrate materials is critical in materials science. Significant efforts are being made to create substrate materials for high-temperature superconductors. Dielectric materials with high-quality factors are being used as superconducting substrate materials and as dielectric resonators due to their ability to filter frequencies selectively. The quality factor of dielectric resonators determines their frequency selectivity. To achieve significant size reduction and stability of resonators, it is essential to have a high-quality factor, high relative permittivity, and low-temperature coefficient of resonant frequency.

In the present work, a modified combustion technique synthesized $RAlO_3$ (R=Gd, Nd, Sm, Pr, and Dy) perovskites, and the microwave dielectric properties were analyzed using the standard resonant method. We measured sintered specimens using an X-band scalar network analyzer (Aeroflex). The permittivity was determined using the Hakki-Coleman method, identifying the TM_{010} mode with an in-house post-resonator test fixture. Dielectric loss and quality factor were evaluated using the cavity-loaded method with $TE_{01\delta}$ mode. We assessed thermal drift by thermally treating the sample-loaded test fixture in a temperature-controlled chamber (hot and cold). We recorded frequency variations and calculated the temperature coefficient of resonant frequency (τ_f) using the TM010 mode over 300°C to 900°C. The temperature coefficient of resonant frequency (τ_f) was also estimated. Materials must have a minimal temperature coefficient of resonant frequency (τ_f), ideally below ±10 ppm/°C, to be used as dielectric resonators. However, the rare-earth aluminates studied in this research show significantly negative τ_f values. To use these materials as dielectric resonators, their τ_f needs to be adjusted. Fortunately, the substantial negative τ_f observed in these compounds is not a significant issue.

G1- 0019

High-Efficiency Microwave Absorbing Materials for Enhanced Stealth Capabilities

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Abstract

In recent time, Stealth technology has become crucial focus in Defence and aviation sectors. Developing cutting-edge absorber materials plays a key role in enhancing stealth by absorbing electromagnetic waves, reducing radar cross-sections, and making objects less detectable. In this study, we have synthesized a multi-layered composite structure by high energy ball milling technique, exhibiting a room-temperature cubic structure. The present analysis was further supported by Raman spectra. The advanced multi-layered composite structure makes reflection and scattering as low as possible. In addition, the work describes lightweight flexible absorber systems that can fit onto a wide range of platforms without loss of aerodynamic performance. Besides, this material system is designed for long-term thermal stability and environmental durability. The reflection loss (RL) of the developed absorber systems demonstrates superior microwave absorption performance. Our experimental results indicate that these absorber systems have the potential to serve as effective microwave absorbers, offering strong absorption, wide bandwidth, a thin profile, and minimal filler content.

G1- 0020

Magnetic Spring Exchange Coupling between Barium Hexaferrite and Nickel Ferrite Flexible Thick Films with PVDF as Polymer Matrix

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Abstract

Ferrites, which are ceramic compounds consisting of iron oxide (Fe_2O_3) mixed with other metal oxides, exhibit a variety of magnetic properties. In particular, ferrites such as barium hexaferrite ($BaFe_{12}O_{19}$) and nickel ferrite ($NiFe_2O_4$) are often commonly used in composite materials where there is an interaction between hard and soft magnetic phases. In the present study, we fabricated highly flexible, free-standing thick film tapes of $BaFe_{12}O_{19}$ and $NiFe_2O_4$ with PVDF as the polymer matrix by the tape casting method. To confirm the phase formation of the final products, $BaFe_{12}O_{19}$ and $NiFe_2O_4$ thick films were characterized by X-ray diffraction. To produce the three-layer laminates, they were stacked and carefully pressed together at 50 - 60 ^{0}C to form a three-layer laminate of hard-soft-hard and soft-hard-soft phases. Both in-plane and out-of-plane MH hysteresis loops of hard-soft-hard (HSH) and soft-hard-soft (SHS) three-layer tapes were recorded using a VSM. The hysteresis loop is characterized by a narrowed middle section, which confirms the low exchange coupling between the layers. The coercivity values were higher ($H_{c\perp}$=1425 Oe, $H_{c\parallel}$ =1078 Oe) in out-of-plane MH loops. However, the remanent and saturation values ($M_{r\parallel}$ =13.79 emu/g, $M_{r\perp}$= 11.06 emu/g, and $M_{s\parallel}$ =38.34 emu/g, $M_{s\perp}$= 33.47 emu/g) are higher in the in-plane MH loops. Higher magnetic properties were observed in the three layer - HSH stacked laminates than in SHS. The magnetic stability of the tapes makes them suitable for advanced magnetic and magnetoelectric applications.

G1- 0021

Comprehensive Analysis of Telluroborate Glasses doped with Nd3+ rare earthions: Exploring the Thermal, Structural, Optical and Physical Characteristics

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Abstract

In the present study, Nd3+ rare earth ion-doped telluroborate glass samples were synthesized using melt quenching techniques. The samples were characterized through various techniques, including XRD, TGA, FTIR, Raman, Optical absorption, photoluminescence, and decay curve analysis. All samples exhibited an amorphous nature in the XRD spectra. The TGA thermograms revealed the thermal behavior, while FTIR and Raman spectroscopy confirmed the coexistence of trigonal BO3 and tetrahedral BO4 units. The optical absorption spectra were recorded at room temperature in wavelength range 180 nm to 1000 nm. The near infrared emission spectra recorded with 808nm laser diode excitation for different concentrations of Nd3+ ions and the emission for the 4F3/2 → 4I11/2 transition at 1060 nm found to be high intense. Judd-Ofelt intensity parameters were determined and spectroscopic parameters were calculated. The study investigated the impact of Nd2O3 concentration on physical parameters. Results showed an increase in density, molar volume and refractive index with higher Nd2O3 concentration, leading to more non-bridging oxygen in the glass matrix. In conclusion, this study provides insights into the potential applications of Nd3+ doped telluroborate glass in advanced optical and photonic devices, contributing to the field of glass science and materials engineering.

Keywords – TGA, FTIR, Raman, Optical properties and Judd-Ofelt intensity parameters.

G1- 0022

Structural and Optical Properties of Rare Earth (Gd) Doped Co-Mg FerriteNanoparticles

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Abstract

Nanocrystalline Gd3+-doped Co–Mg ferrite nanoparticles with the chemical formula Co0.5Mg0.5Fe2−xGdxO4 (x = 0.0 to 0.10, in step size of 0.02) were prepared via sol-gel self-ignition route. The impact of Gd3+ ion doping on structural, electronic, and magnetic properties of Co- Mg ferrites has been studied. Rietveld refinement of X-ray diffraction (XRD) results confirmed the formation of single-phase, highly crystalline cubic spinel structure in the space group Fd3 m with crystalline size in the range of 20-80 nm. The Fourier transform infrared rays (FTIR) spectrum shows that the samples have a broad range of chemical interactions. UV-Vis absorbance results show that the band gap energy of Co0.5Mg0.5Fe2O4 nanoparticles decreases
with increasing Gd3+ ion doping.

Keywords Co0.5Mg0.5Fe2−xGdxO4, Nanoferrites, XRD, Rietveld refinement, FTIR, UV-VIS.

G1- 0023

Giant energy-storage density with ultrahigh efficiency in lead-free $0.94NaBiTiO_3$-$0.06BaTiO_3$ Bulk ceramics

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Abstract

Lead free polar materials/electro ceramics received tremendous attention now a days due to its wide range of applications in current generation of electronic industries. This polar material especially, in energy applications shows the path breaking identity because of its structural and electrical improvement by modifying the fingerprint ABO_3perovskitestructures. The present report focuses to address the above affirmations with help of lead free $NaBiTiO_3$-$BaTiO_3$. Here, the structural existing of this specimen address with help of structural refinement with quantitative phase contribution. The giant energy-storage density W_{rec} ≈2.34J.cm^{-3}, high efficiency η ≈93% and excellent thermal stability. The substitution of rare earths facilitates the refine grain growth dielectric strength and increases the resistivity of $NaBiTiO_3$-$BaTiO_3$.The current work provides a new solution to successfully design next-generation pulsed power capacitors by fully utilizing relaxor ferroelectrics in energy-storage efficiency and thermal stability.

G1- 0024

Cr_2O_3-Al_2O_3 Binary Thin Films: A Study on Enhanced Electrochromic Properties

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Abstract

In recent years, electrocromic devices based on metal oxides have emerged as promising candidates for smart windows in energy-efficient buildings, variable-reflective mirrors, information displays, and other cutting-edge applications. Electrochromic smart windows (ESWs) automatically modify their transparency in response to environmental conditions, controlling how much solar energy enters the building. This helps create a comfortable indoor atmosphere by managing light and heat levels. Numerous transition metal oxides are known to exhibit electrochromism. Among them, chromium oxide (Cr_2O_3) is one of the important but less-studied oxides. Despite its potential in electrochromic applications, Cr_2O_3 has not received as much attention as more widely used materials like tungsten oxide (WO_3), which offers stronger optical contrast, faster switching speeds, and superior overall electrochromic performance To enhance the electrochromic (EC) performance of Cr_2O_3, we developed an indigenous high-purity sputtering target from equally mixed powders of Cr_2O_3 and Al_2O_3. Using this target, thin films were deposited via the RF magnetron sputtering technique onto fluorine-doped tin oxide (FTO) coated substrates, applying varying RF powers of 100, 200, and 300 W. Interestingly, the thin films produced from this Cr_2O_3-Al_2O_3 binary system demonstrated significantly improved optical modulation, faster switching response times, and enhanced cycling stability. As a result, electrochromic devices based on this Cr_2O_3-Al_2O_3 combination are more suitable for practical applications such as smart windows, where high durability, energy efficiency, and excellent performance are critical.

G1-0025

Comparative Study on the Mechanical and Tribological Behavior of Aluminum 6061 and Al 5083 Composites Reinforced with SiC, Co, Cu, and Ni Particulates

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Abstract

This study compares the mechanical characterization of Al6061 and Al5083 alloys when reinforced with various particulates, specifically silicon carbide (SiC), cobalt (Co), copper (Cu), and nickel (Ni). Both alloys are widely utilized in automotive and aerospace applications, but they exhibit distinct characteristics that influence their performance in composite form. Aluminum 6061 is known for its good corrosion resistance, weldability, and moderate to high strength, making it suitable for structural applications. In contrast, Al 5083 is a high magnesium alloy renowned for its excellent weldability and resistance to marine environments, though it typically has lower wear resistance compared to 6061. This research investigates the effects of particulate reinforcement on the mechanical properties, such as hardness, tensile strength, and impact resistance, as well as the tribological behavior of the composites under different wear conditions, including sliding wear and air erosion. Experimental results demonstrate that the addition of 3% wt of SiC and Co significantly enhances the mechanical properties of aluminum 6061-based MMCs, yielding increased hardness and tensile strength. Meanwhile, the Al 5083-based composites exhibit improved hardness with the incorporation of copper and nickel, with optimal performance noted at 3% wt of Ni and Cu. However, the ultimate tensile strength and flexural strength were found to be highest in the Al 5083 composite with 0% wt of Ni and 3% wt of Cu. Overall, this comparative analysis reveals that while both aluminum alloys benefit from particulate reinforcement, their differing base properties lead to distinct performance outcomes in composite form. Understanding these differences is crucial for selecting appropriate materials for specific applications in demanding environments.

Keywords: Aluminium, Copper, Nickel, Cobalt, Silicon Carbide, Metal Metrix Composites.

G1-0026

Advancing Luminescent Capabilities and Achieving Efficient Multicoloured and Controllable White Photo luminescence through Erbium and Holmium ions Doping in Yttrium Alumina Bismuth boro Silicate Glasses

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Abstract

This research examines the emission properties of Erbium (Er3+) and Holmium (Ho3+) ions
from Yttrium Alumina Bismuth boro Silicate glasses (YAlBiBSi) in the near UV and visible
regions, with the aim of furthering high-performance optical systems. A primary issue that is tackled is the enlargement of the color gamut of the display, which is complicated by the need to individually adjust the proportions of light emitted at different wavelengths. To circumvent this, the research incorporates Er3+ and Ho3+ ions into the YAlBiBSi matrix via a doping process, which generates variegated emissions with a narrow full width at half-maximum and high Photo luminescence quantum yields (PLQYs). It is important to note that the blue emission, which extends 450-480 nm, belongs to holmium. On the other hand, the narrowband green (530-552nm) and red (622-655nm) emissions primarily stem from Ho3+ and Er3+ ions, respectively.It is emphasized that efficient energy transfer between numerous luminescent centers is a crucial element in producing such tunable and efficient emissions. The systematic modulation of emission color is achieved by the study through control of the RE3+ doping level. Specifically, adjustable white-light emission is achieved between 10308 K (0.276, 0.285) and 4610 K (0.348,0.301). The outcomes not only serve as a source of inspiration for material development but also highlight the considerable potential of these glasses in various fields—including sealants, nuclear waste immobilization, optoelectronics, solar energy technologies, softening temperature, chemical resistance, low thermal expansion, dispersion, and mechanical strength as a result of their exceptional properties.

G2- 0001

Integrating Remote Sensing and Field Survey for Vegetation Classification Based on Chlorophyll Content Using NDVI and Random Forest Techniques

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Abstract

Vegetation classification based on chlorophyll content provides critical insights into plant health and ecosystem sustainability. This study combined satellite-based analysis and field survey data to classify vegetation around the region at latitude 19.00445 and longitude 75.376804. Sentinel-2 satellite imagery from the European Space Agency was processed using SNAP software to calculate the Normalized Difference Vegetation Index (NDVI), an established indicator of vegetation health. The NDVI values were used to classify vegetation based on its chlorophyll content. Concurrently, a field survey was conducted to collect crop samples from the same location. Chlorophyll content was measured in the laboratory for the collected samples to validate the NDVI-derived classifications. A Random Forest classification technique was applied to the processed imagery for detailed vegetation mapping. This integrated approach of remote sensing data and ground truth analysis enabled accurate classification of vegetation types based on their chlorophyll content. The study demonstrates the effectiveness of using SNAP software and NDVI analysis for monitoring vegetation health and offers a scalable method for assessing large agricultural areas. The results have significant implications for improving agricultural practices, monitoring ecosystem changes, and optimizing land use management.

G2- 0002

Investigating Newton's Law of Cooling for Fluids and Granular Solids: A Regression-Based Model Fitting Approach

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Abstract

Cooling of a fluid in a laboratory set-up follows the Newtonian cooling mechanism having exponential decay as the signature curve. The given curve models the cooling process as a single order exponential decay. In the present study, we investigate the cooling rates of fluids commonly encountered in daily life, such as water, milk, mustard oil and of granular solids like sand. MAX6675 module with K-type thermocouple interfaced with Arduino is used for acquisition of temperature data. Computational approach used to model the experimental data utilizes the techniques of **curve fitting**, **data splitting (training and validation sets)**, and **residual error analysis.** The given data set in each case is divided into two parts with 80% of data being used for training the model and the rest 20% for validating it. Residuals are computed and analyzed to assess the quality of the fit and identify any systematic patterns that might indicate overfitting or underfitting. By comparing the training and validation errors, the generalizability of the model is evaluated. Our results indicate that a double exponential decay model provides a better fit with lower values of residual errors in all cases, thereby, capturing the nuances of the cooling process more accurately. The study highlights the role of data visualization and residual analysis in refining the model and ensuring the fidelity of the fitted parameters, the respective cooling rates in each case. This methodology offers a robust framework for analyzing thermal processes and can be extended to other experimental setups involving heat transfer.

G2- 0003

DNA Bases Interaction with Polycyclic Aromatic Hydrocarbons as Finite Size Model of Graphene

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Abstract

DNA bases (adenine, guanine, cytosine and thymine) and base pairs interaction with polycyclic aromatic hydrocarbons (PAHs) as finite size models of graphene were investigated theoretically using the Density Functional Theory (DFT). The finite size PAHs were optimized in a plane as finite size models of graphene. All the bases and base pairs were studied with finite size PAH at the B3LYP, B98 and MPW1PW91 functionals of DFT along with the 6-31G(d,p) basis set. To find the more feasible reaction sites, binding energies were calculated at all the mentioned level of theory. The calculated binding energies reveal that edges of PAHs are more feasible for reactions.

Keywords: Graphene, Polycyclic aromatic hydrocarbons, DNA bases and base pairs, Electron density

G2- 0004

Strain Induced Alterations in the Thermoelectric Properties and Room Temperature Thermal Expansion Behaviour of 2D SiH and GeH Monolayers: an account from First-Principles DFT and Molecular Dynamics Calculations

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Abstract

The present study is focused to understand the strain driven modulations in thermoelectric properties and room temperature thermal expansion behaviour of 2D SiH and GeH monolayers from first-principles DFT and molecular dynamics calculations [1]. Electronic band structures and the associated thermoelectric properties of the compounds under ambient and external strains have been explored in terms of Seebeck coefficients, electrical conductivities, power factors and electronic thermal conductivities. The phonon dispersion relations have been investigated to estimate the lattice thermal conductivities (κ_l) of the systems. The Grüneisen parameter (γ) is also calculated to consider the phonon anharmonicity of the systems. It is found that γ varies over a wide range between its positive and negative channels and the negative γ represent the negative thermal expansion (NTE) behaviors of the monolayers. Closer observations on the temperature dependent lattice parameters and linear thermal expansion coefficients of the systems suggest close involvements of the crystallographic "a (= b)" axis towards their NTE behaviours. The thermoelectric figure of merits (ZT) of SiH and GeH monolayers under ambient and external strains have been explored from the collective effects of the aforementioned parameters. Estimations of κ_l and ZT further reveal that both SiH and GeH monolayers show minimum κ_l (0.55 and 0.69 $Wm^{-1}K^{-1}$) and maximum ZT (1.26 and 0.81) at -2% compressive strain. This study will be helpful in exploring the strain induced responses of SiH and GeH compounds which in turn may bear potential applications in clean and global energy conservation, aerospace engineering, thermal-expansion compensators and high-precision devices.

G2- 0005

Optimization of Link Distance and Receiver Parameters for Efficient Underwater Communication Using Monte-Carlo Simulation

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Abstract

In this paper, the propagation of a 532nm Gaussian laser beam with ±6 mrad divergence in various underwater environments, specifically pure sea, Clear Ocean, and coastal water is analyzed using Monte Carlo simulations. The spatial distribution of the laser beam is investigated at different link distances to find the design of efficient underwater communication systems. Results indicate that a tailored approach to system design is crucial for optimal performance. Specifically, it is essential to minimize the divergence angle of the light source, and determine optimum link distance and receiver diameter for any specific type of water. For instance, our simulations show that for a 50m transmission distance in pure sea and clear ocean water, a receiver diameter of 0.6m is optimal, while coastal water limits link distance to 30-40m, requiring adjusted system parameters. Moreover, our findings provide valuable insights into the allowable deviation from line-of-sight configuration, enabling the quantification of detector misalignment tolerance. This knowledge facilitates the design of robust underwater communication systems that can accommodate spatial variability and movement. Our research highlights the importance of balancing light source characteristics, link distance, and receiver design to minimize signal loss and maximize system performance, ultimately contributing to the development of more efficient and reliable underwater communication systems.

G2-0006

Surface plasmon resonance biosensor for identification of Breast cancer under optimum radiation damping condition

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Abstract

Over the last few decades SPR-Surface Plasmon Resonance based sensors have advanced applications in chemical sensing, material characterization and biosensing. Cancer is a type of chronological disease detection of which at an early stage is challenging task. Breast cancer is the most life-threatening disease among women which is about 2 million surveyed in 2020, so detection of which becomes quite important at starting phase. In this a hybrid design and simulation-based analysis of SPR biosensor for breast cancer Detection is being implemented. The designed sensor structure consists of (CaF2 prism/Ag /Si_3N_4/AM) at a wavelength of 1000 nm. Silicon nitride (Si_3 N_4) is a rather costly material, but in applications where it may surpass commonly used materials with long life and very dependable low maintenance operation, its performance to cost benefit ratio is good. Using 2D simulation technique, the figure-of-merit (FOM) of the sensor is optimized by simultaneously varying the thickness of Ag layer (d_M) and Si_3N_4 layer (d_A) under optimum radiation damping (ORD). An optimized FOM as high as 3670 RIU^{-1} (at d_M = 32.6 nm) has been achieved corresponding to d_A = 3.3 nm. At ORD, the corresponding power loss ratio (PLR) is as high as 4.078. The proposed application of Si_3N_4 in a plasmonic sensor utilized under ORD conditions significantly improves sensing performance and has been investigated as the most effective method for detecting breast cancer. As this material has its advantage of large refractive index and transparent behaviour in nearby infrared region.

H1- 0001

Investigating the Interaction between Cyclo[12]carbon and Graphene Quantum Dot: A First-Principles Study

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Abstract

In this investigation, we explore the interaction between Cyclo[12]carbon (C_{12}) and Coronene Graphene Quantum Dot ($C_{24}H_{12}$), two zero-dimensional carbon-based nanomaterials characterized by their unique structural and electronic properties. Our study consists of an in-depth analysis of their structural, electronic, and spectroscopic properties to determine the nature of their interaction. The final separation between the C_{12} nanocluster and Coronene GQD is found to be 3.38 Å, indicative of the close proximity. Importantly, minimal alterations in bond length and bond angle signify a van der Waals interaction. Furthermore, the negative formation energy and the all positive frequencies in the IR spectra provide compelling evidence for the stability of the newly formed complex. This underscores the thermodynamic favorability of this complexation through the interaction between C_{12} and GQD, highlighting their potential for various applications in nanotechnology and materials science.

Keywords: Cyclo [12] carbon, Graphene Quantum Dot, Density Functional Theory; Interaction Mechanism.

H1- 0002

Study on structural, magnetic, and thermoelectric properties of Fe2+xNi 1-xTi (x=0, 0.25, and 0.5) based intermetallics: A first principles DFT study

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Abstract

The structural, electronic, thermoelectric, and magnetic properties of the series of Heusler alloys Fe2NiTi and its Fe*2*+*x*Ni*1*-*x*Ti (*x*=25, 0.5) have been investigated theoretically. Here, we primarily concentrate on the thermoelectric characteristics and magnetic properties of this new class of Heusler compounds, known as all-3d Heusler alloys. A2BTi type alloys of Fe2NiTi and its Fe (Iron) excess in Ni (Nickel) sites like Fe*2*+*x*Ni *1*-*x*Ti (*x*=0.25,0.5) were studied using Density Functional Theory (DFT) and predicted the electronic structure and thermoelectric properties. The first principles calculations are based on the full potential linearized augmented plane wave (FP-LAPW) method implemented in the WIEN2k code. The electronic structure shows the material is metallic. DFT studies using Wien2k show a magnetic moment of 3.84 μB, 9.03 μB, and 17.2 μB, (this is too high, and some mistake is there. Make it per formula unit) respectively, highlighting the increase in the magnetic moment with Fe addition. The Seebeck coefficient (S) is found to increase and the thermoelectric power factor is found to decrease with Fe addition on the Ni sites due to the increase in thermal (κ) and electrical conductivities (σ).

H1- 0003

Preparation of 4-Hydroxy-3-((4-hydroxy-2-oxo-2H-chromen-3-yl) (2,3-dimethoxyphenyl)methyl)-2H-chromen-2-one molecule: Structural, Optical and Thermal studies using DFT

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Abstract

In this report, a facile and efficient protocol has been followed for the synthesis of novel 4-Hydroxy-3-((4-hydroxy-2-oxo-2H-chromen-3-yl)(2,3-dimethoxyphenyl)methyl)-2H-chromen-2-one via a one pot reaction of aryl aldehydes with 4-hydroxycoumarin and in the presence of ethanol at 800C. The synthesized molecule is being further tested for structural confirmation with nuclear magnetic resonance and Fourier transform infrared spectroscopic technique. From the obtained result of 1H NMR spectroscopy it has been confirmed that the synthesized molecule is stable with ten electron signal. The optical absorption measurement was carried out using density functional studies in order determine the optical property of the synthesized molecule such as the bandgap and molar extinction coefficient. Further the bond angles and bond lengths of the molecule The theoretical calculated conceptual DFT descriptors of complexes of the titled molecule has been estimated. From over all outcomes the molecule exhibited a considerable result in order to derive the optical device application.

Keywords: Synthesis, Aldehydes, Structure.

H1- 0004

Optoelectronic Properties of Homo-bilayer of $YBiSe_3$: A First-principles Study

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Abstract

In this work, the van der Walls (vdW) homo-bilayer of $YBiSe_3$ is constructed. The $YBiSe_3$ homo-bilayer shows honey-comb stable structure with semiconducting behavior. This homo-bilayer were studied using GGA-PBE and hybrid HSE06 functional. It shows semiconductor behavior with band gap of 0.62 eV from PBE functional. The negative cohesive energy of bilayer confirms the energetic stability. The partial density of states (PDOS) has been calculated for $YBiSe_3$ homo-bilayer to gain the insight into the orbital contribution. The absorption spectrum indicates extensive coverage in electromagnetic spectrum. Absorption is observed in visible and UV region, and small absorption is observed in IR region. This confirms its effectiveness in nano-optoelectronic devices and its applications.

H1- 0005

Sc_2CF_2 MXene as a Promising Material for Formaldehyde Storage

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Abstract

Formaldehyde (HCHO) is a colorless gas with a strong odor that poses significant health risks to humans. Considerable efforts have been invested in minimizing the concentration of gaseous formaldehyde in indoor environments. This study predicts F-terminated 2D MXene monolayer; Sc_2CF_2 as an effective adsorbent of formaldehyde using the Density Functional Theory. The Sc_2CF_2 monolayer is a suitable candidate for the effective adsorption of HCHO, showing an adsorption energy of 0.40 eV per molecule and the highest adsorption energy achieved for possible maximum HCHO adsorption on the monolayer is 0.65 eV. This moderate adsorption energy suggests that Sc_2CF_2 is a suitable material for removing formaldehyde from indoor air. To determine the adsorption stability at room temperature, an Ab-initio Molecular Dynamics simulation has been performed, which confirms the stability of adsorption at 300 K. Moreover, high adsorption capacity is predicted for the Sc_2CF_2 adsorbent.

H1- 0006

Ag Functionalized $GaAlTe_2$ Monolayer as a Promising Gas Sensor for Detecting Asphyxiating Gases

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Abstract

Asphyxiating gases, such as carbon monoxide (CO), hydrogen sulfide (H_2S), and methane (CH_4), are a serious threat to human health. These gases displace oxygen from the air, causing suffocation and other serious respiratory distress. Thus, the detection of these gases is crucial to ensure human health and safety. In this work, the sensing mechanism of Ag-functionalized $GaAlTe_2$ monolayer (ML) has been investigated using a density functional approach to detect asphyxiating gases such as CO, CH_4, and H_2S. The adsorption properties are obtained by calculating absorption energies, charge transfer, electronic characteristics, and recovery time. The notable modifications in the band structure and partial density of states (PDOS) suggest the successful detection of these gases. The suitable values of adsorption energies and recovery time in seconds indicate that the Ag-$GaAlTe_2$ ML successfully detects the gases CO and H_2S. The results validate that the Ag-$GaAlTe_2$ ML is a promising gas sensor for detecting asphyxiating gases (CO, CH_4, and H_2S).

H1- 0007

First-principle Investigation of $ZrCl_2$ Monolayer as a Promising Na Host Material

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Abstract

Na-ion batteries (SIBs) have gained significant attention for their eco-friendly nature, low-cost and wide availability in nature. This study explores the electrochemical and electronic properties of $ZrCl_2$ monolayer (ML) as SIBs using Density Functional Approach. The electronic properties shows that $ZrCl_2$ ML has an indirect bandgap of 1.00 eV, confirms its semiconducting nature. Moreover, Na adsorption on $ZrCl_2$ ML leads to its metallic properties. The calculated adsorption energy indicates the significant adsorption strength for Na, suggesting that the electrochemical interaction between the $ZrCl_2$ host and Na ions is favorable. As the Na concentration increases, material's electronic conductivity also improves. The Na storage capacity of 535.89 mAh/g is achieved, along with an average OCV (open-circuit-voltage) of 0.662. Therefore, the results indicate that $ZrCl_2$ ML is a promising candidate for SIBs.

H1- 0008

Study of Elastic Anisotropy of Compounds RhBiX (X=Hf, Ti and Zr)

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Abstract

The study shows the minimum and maximum values of Young's modulus, Poisson's ratio and shear modulus of compounds RhBiHf, RhBiTi and RhBiZr at zero pressure using ELATE software. Anisotropy parameters A_G and A^U for RhBiTi are slightly greater than the respective values of these parameters for RhBiHf and RhBiZr. The ratios of maximum to minimum values of Young's modulus (E_{max}/E_{min}), linear compressibility (β_{max}/β_{min}), shear modulus (G_{max}/G_{min}) and Poisson's ratio (ν_{max}/ν_{min}) for RhBiTi are 1.12, 1.00, 1.14 and 1.26, respectively. The investigation shows the spatial dependence of Young's modulus, linear compressibility, Poisson's ratio and shear modulus of compound RhBiTi through polar plots.

H1- 0009

Electronic property of full heusler alloys Ac2AgPb: First Principe calculations

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Abstract

In this study, we investigate the electronic properties of the full Heusler compound Ac_2AgPb using first-principles methods based on density functional theory (DFT). Full Heusler alloys are known for their versatile electronic characteristics, making them promising candidates for applications in spintronics, thermoelectrics, and magnetoelectronics. The structural stability of Ac_2AgPb is confirmed through optimization of the crystal structure in its cubic L21 phase. The electronic band structure, density of states (DOS), and charge density distribution are systematically explored to reveal the nature of the band gap and electronic conduction properties. Our results indicate that Ac_2AgPb exhibits metallic behavior with a zero band gap of [X eV] at the [Γ-point/other high-symmetry points]. The contribution of the constituent atoms to the electronic states near the Fermi level is analyzed, showing that [Ac/Ag/Pb] states play a dominant role. This theoretical investigation provides valuable insights into the potential applications of Ac_2AgPb in electronic and thermoelectric devices.

H1- 0010

Theoretical study of static and dynamic equation of states of cerium and ytterbium

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Abstract

Theoretical study of the dynamic equation of state or shock Hugoniot plays a key role in describing behaviour of materials under simultaneous high temperature and high pressure that are very difficult to achieve in the experiments. Schock Hugoniot is locus of all possible states that arises due to a single shock from a given initial state, generally explained by thermodynamic variables like pressure, volume and internal energy or enthalpy. Anharmonicity aroused due to lattice ions and thermally excited electrons should be accounted properly at such high temperature and high pressure. In the present study, a conjunction scheme of a local form of the pseudopotential proposed by Krasko and Gruski (KG) and mean field potential (MFP) has been used to account anharmonic effects due to lattice vibrations. The anharmonicity due to thermally excited electrons has been included using Mermin functional. Static as well as dynamic equation of state along with temperature along principal Hugoniot of rare earth elements cerium and ytterbium has been studied theoretically. The conjunction scheme is found to be capable to account for anharmonicity at extreme environment such as high temperature and high pressure.

H1- 0011

Harnessing Machine Learning for Comparative Analysis of Nanomaterials in Agro-environmental Applications

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Abstract

The integration of nonmaterial (NM) and machine learning (ML) presents transformative opportunities in addressing NM insights and critical global challenges such as agriculture sustainability and climate change mitigation. This study conducts a comparative analysis of various nonomaterial and their applications in agriculture and environmental change. By leveraging ML techniques, we can predict and optimize the properties and functionalities of these nonomaterials to enhance their effectiveness in specific applications. In agriculture, nonomaterials are employed in the development of nanofertilizers, nanopesticides, nanobiosensors and nanosensors. This will contribute to improving the quality of crop yield, pest control and soil health monitoring. In the environment, nonomaterials are employed in the development of nanofilters for environmental and climate change effects related issues. Machine learning (ML) and nonmaterials (NM) are increasingly intersecting to drive advancements in various fields. ML model facilitates the precise tuning of nonmaterial properties to maximize their efficiency and minimize environmental impact.

This comparative analysis underscores the potential of combining NM and ML to drive innovations in agro-environmental solutions. It highlights the importance of interdisciplinary approaches in developing sustainable technologies that address agro-environmental issues. By leveraging advanced machine learning algorithms and artificial intelligence (AI), we analyze data from nanosensors and nanomaterials to improve their specificity, sensitivity and accuracy. This approach solves critical challenges such as food security and environmental conservation but also paves the way for innovative AI solutions as smart agro-environmental applications.

H1- 0012

DFT study of $TmGa_3$ Intermetallic Compound

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Abstract

Intermetallic alloys and compounds of transition metal elements fall into an interesting category of materials with a large number of technological applications. These materials gain attention because of their exotic mechanical, electronic and magnetic properties (Watson and Bennett 1978). The cubic intermetallic compound $TmGa_3$, which crystallize in $AuCu_3$ structure as shown in the Figure 1, is interesting because of its relatively strong quadrupolar pair interactions. In the present work we have investigated the structural, electronic, elastic and mechanical properties of isostructural and isoelectronic magnetic $TmGa_3$ intermetallic compound, by using first principles density functional theory based on full potential linearized augmented plane wave (FP-LAPW) method. The calculations are carried out within LSDA for the exchange correlation potential. Our calculated ground state properties such as lattice constant (a_0), bulk modulus (B) and its pressure derivative (B') are in good agreement with the available experimental and other theoretical results. The computed electronic band structure and DOS reveal that the compound is metallic in nature. We also predicted the elastic constants and mechanical properties for this compound using LSDA approximation. The compound is found to be brittle in nature in accordance with Pugh's criteria.

H1- 0013

HOMO-LUMO Insights into Charge Transfer and Energy Properties of ZnTCPP Complexes

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Abstract

This study employs Density Functional Theory (DFT) calculations to investigate the optoelectronic potential of Zinc 5, 10, 15, and 20-tetrakis(4-carboxyphenyl) porphyrin (ZnTCPP). We analyze the energy states and charge transfer properties of ZnTCPP, focusing on the electronic characteristics derived from HOMO-LUMO and energy bandgap (ΔE) analyses. We focus on how the metallic and its pure equivalent, TCPP, exhibit distinct charge transfer behaviours.

On comparison of the multiple global chemical reactive descriptors (GCRD), such as maximal charge transfer, ΔN_{max}, an important outcome is revealed. A greater ΔN_{max} value indicates that metallic TCPP is more reactive than pure TCPP because of inherent property of metallic TCPP. The rate of charge transfer increases in metallic TCPP while it decreases in pure TCPP. According to our findings, metallic TCPP exhibits higher reactivity and charge transfer, which makes it a viable option for a variety of optoelectronic uses, including optical switches, sensors, and power regulators.

Furthermore, the newly identified characteristics of metallic TCPP highlight opportunities for developing customized porphyrins in advanced devices with finely tuned optoelectronic capabilities. Overall, this research deepens our understanding of the complex interactions between metallic and pure porphyrin structures, paving the way for innovative applications in the field.

H1- 0014

Effects of Arsenic Doping (As) on Structural and Electronic Properties of Zigzag Germanium Sulphide Nanoribbons: A First-Principles Approach

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Abstract

Density functional theory (DFT) is employed to study the structural and electronic of zigzag germanium sulfide nanoribbons (ZGeSNR) via substitutional doping of Arsenic (As-) atom (p-type impurity). We observed the effect of Arsenic (As) doping on the Ge-edge, S-edge, and center of ZGeSNR. Post substitutional doping structural stability of the doped structures was evaluated via. Formation energy calculation and we found that all the configurations were thermodynamically stable. Further, we have also calculated the electronic properties on the basis of the E-k diagram and density of state (DOS) profile, which shows that the pristine nanoribbons turn metallic upon doping. This induced metallicity in ZGeSNR warrants their applicability in the field of 1D nano interconnects.

H1- 0015

Analysis of Electronic and Thermoelectric Response of Germanium Based Perovskite Halide: Potential Material for Device Application

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Abstract

The structural, electronic and thermoelectric properties of Cesium Germanium halides $CsGeX_3$ (X= Br and I) have been examined using density functional theory with the generalized gradient approximation (GGA) in cubic phase. The structural properties such as lattice parameter (a_0), bulk modulus (B) and its pressure derivative are found to be good agreement with the available experimental and theoretical results. The electronic properties have been analyzed from band structure and density of states (DOS) which reveal that both the compounds show semiconducting nature with direct band gap at R-point. The values of energy band gap (Eg) are also show good agreement with previously data. The thermoelectric behavior has been explored in terms of electrical conductivity (σ/τ), electronic thermal conductivity (κ_e/τ), Seebeck coefficient (S) and power factor ($S^2\sigma/\tau$). The higher values of Seebeck coefficient suggest that all the compounds are n-type semiconductors. The values of power factor increase with increasing temperature.

H1- 0016

A DFT Approach to Structural, Electronic, and Thermodynamic Properties of Binary Rare-earth Nitrides REN (RE = Pr & Nd)

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Abstract

In the present work, we apply density functional theory (DFT) with the PBE (Perdew–Burke–Ernzerhof) and WC (Wu–Cohen) exchange-correlation functionals using the generalized gradient approximation to investigate the structural, electronic, and thermodynamic properties of binary rare-earth nitrides REN (RE = Pr and Nd) compounds. Our computed structural parameters, such as equilibrium lattice constants, bond angles, and bond lengths, show excellent agreement with both experimental and previous theoretical results. The electronic properties of praseodymium and neodymium nitrides are examined through electronic band structure and density of states analyses. The calculations of the second order elastic constants (Cij) and the resulting elastic moduli, including bulk modulus (B), shear modulus (G), Young's modulus (E), Poisson's ratio (ν), and the B/G ratio, are also reported and analyzed. Additionally, we compute thermodynamic properties using the quasi-harmonic Debye model. This study provides a valuable basis for further experimental and theoretical exploration of the potential applications of these materials.

H1- 0017

A DFT-Based Comparative Study on the Structural, Magnetic, Electronic, and Thermoelectric Properties of $TMCo_2$ (TM = Ti, Nb) Intermetallics

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Abstract

In this work, we present a comparative study of the structural, magnetic, electronic, and thermoelectric properties of cubic binary Laves-phase intermetallic compounds with the general formula $TMCo_2$ (TM = Ti, Nb), using density functional theory (DFT) within the Wien2k code. Geometrical optimization, performed through the Birch-Murnaghan equation of state, shows excellent agreement with prior theoretical and experimental findings. The magnetic properties confirm the presence of ferromagnetic ordering. To explore the electronic properties, we have analyzed the band structures and density of states. Thermoelectric behavior is investigated using the BoltzTrap code, based on Boltzmann transport theory. Furthermore, the influence of chemical potential on the Seebeck coefficient and power factor is evaluated at temperatures of 300, 600, and 900 K.

H1- 0018

Interplay of polymer dynamics and polymer friction in PEO-$NaPF_6$ electrolytes

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Abstract

Sodium ion-based solid electrolytes are replacing conventional Li-based liquid electrolytes due to higher cost-effectiveness, safety, biocompatibility, and mechanical stability. In this study, we have investigated the interplay of polymer dynamics and polymer friction on ion transport and structure properties of PEO-$NaPF_6$ electrolytes due to the effect of different molecular weights of polymer chains using atomistic molecular dynamics simulations. Our results show that the diffusion coefficients of both ions follow different decaying exponents when changing the molecular weight of polymer chains. Furthermore, polymer chain length also affects ionic conductivity and monomeric friction coefficient. These strong correlations of structural and transport properties of the given system with polymer chain length can provide detailed insights into mechanisms governing the transport properties.

H1- 0019

Impact of Spacers on Second-Order Nonlinear Optical Properties of Triphenylamine Chromophore Derivative: A DFT Study

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Abstract

In this study, we designed a novel triphenylamine chromophore derivative S, aimed at nonlinear optical (NLO) applications. We investigated the impact of three distinct spacer groups—S1, S2, and S3—on the NLO properties using density functional theory (DFT) and time-dependent DFT (TD-DFT) in the gaseous phase. Nonlinear optical materials play a crucial role in photonics, with applications spanning optical communication, frequency doubling, electro-optic devices, nonlinear imaging, and sensors. By employing the ωB97XD functional alongside a 6-311++G (d,p) basis set, as it accurately predicted the NLO responses. Our computational analysis revealed significant findings: chromophore S exhibited a dipole moment of 3.34 Debye, a linear polarizability of $96.56718819\times10^{-24}$ esu, and a first hyperpolarizability of $170412.8577\times10^{-33}$ esu. Among the spacers, S3 exhibited superior properties, with a dipole moment of 3.78 Debye, a linear polarizability of $97.22672302\times10^{-24}$ esu, and a first hyperpolarizability of 189455.202×10^{-33} esu. Natural bond orbital (NBO) analysis provided insights into the electron density delocalization, enriching our understanding of NLO behavior. The evaluation of HOMO-LUMO gaps allowed us to connect energy levels with optical activity. Additionally, simulations of UV-Visible spectra further corroborated our findings, emphasizing the absorption characteristics of the designed spacers. These results shed light on the relationship between molecular architecture and optical properties, demonstrating that strategic spacer design can enhance the nonlinear optical characteristics of organic materials. This work advances the rational design of high-performance organic NLO materials and underscores the efficacy of computational methods in predicting and guiding experimental approaches in photonic applications.
Keywords: Organic NLO materials, nonlinear optics, spacer effects, Triphenylamine derivative, DFT

H1- 0020

Electronic, magnetic, optical, thermodynamic and thermoelectric properties of Half Heusler alloy, HfNiSn: First principles Calculations

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Abstract

In this work, half Heusler alloy, HfNiSn were studied via first principles method within the PBE-GGA exchange correlation functional. Pressure and strain effect on different physical properties of the compound has also been studied. Volume optimization curve reveal that, HfNiSn half Heusler compound is more stable in nonmagnetic ordering with gamma-phase of cubic structure (S.G 216). Density of state and band structure calculations indicates the semiconducting behaviour of the compound. Our density of state outcomes shows that HfNiSn is an indirect bandgap semiconductor half-Heusler alloy with a narrow energy gap of 0.33 eV. Calculated formation energy and cohesive energy for the compound predict its thermodynamic stability. Estimated Young's modulus (E), elastic constants (C11, C12 and C44), Shear modulus (G), Poisson's ratio (ν), reveal that compound is mechanical stable and shows ductile behaviour under studied pressure range. Optical properties studied with pressure effects show the slight changes. Absorption spectra show the maximal absorption in the visible and UV region of the electromagnetic radiation which could be utilized as good UV absorbent in the devices. Thermoelectric properties reveal the significance of compound in thermoelectric applications. Overall, all the physical properties reveal its importance as good electronic, elastic, and optical material to be utilized in the future opto-electronic and thermoelectric devices.

Keywords: Half Heusler alloy; semiconductor; optical properties; band structure; density of states

H1-0021

Design and simulation of highly efficient and Stable 2D-3D DJ Perovskite Solar Cell

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Abstract

This paper presents a theoretical investigation of a perovskite solar cell device with the structure **FTO/TiO_2/$CH_3NH_3PbI_3$/$PeDAMA_5Pb_5I_{16}$/Spiro-OMeTAD**. The focus is on the effects of electron transport layers (ETLs) and hole transport layers (HTLs) on optimizing the device's performance, using SCAPS-1D software. Perovskite solar cells (PSCs) have made significant advancements in recent years, but their instability due to moisture remains a major obstacle for commercialization. This has led to the development of 2D perovskites, which offer greater stability due to the incorporation of organic cations and inorganic slabs in an alternating arrangement. There are two types of 2D perovskites: Ruddlesden-Popper (RP) and Dion-Jacobson (DJ) phases, both of which are more stable than traditional 3D perovskites. By merging these two 2D phases, researchers aim to improve both stability and efficiency. The proposed **DJ 2D-3D perovskite solar cells** have demonstrated remarkable performance, achieving a **power conversion efficiency (PCE) of 24.23%**, even when exposed to challenging conditions like **high temperature and moisture**. This level of efficiency, combined with the superior **stability** of 2D-DJ perovskites, makes them a promising alternative for **photovoltaic applications**. Their **open-circuit voltage (V_{OC})** of **1.385 V**, along with a **fill factor (FF) of 79.06%** and **short-circuit current density (J_{SC}) of 22.126 mA/cm^2**, highlights their potential to outperform traditional 3D perovskites, offering both **efficiency and durability** in demanding environments.

H1-0022

Filtered Spectrum Modelling of High-Performance DJ 2D-3D Perovskite Tandem Solar Cell

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Abstract

This paper examines the DJ 2D-3D perovskite tandem solar cell using SCAPS-1D software. The analysis of power conversion efficiency (PCE) has been carried out for $PeDAMA_2Pb_3I_{10}$, with a bandgap of 1.88 eV, and a Pb-Sn-based narrow bandgap halide (NBH), $FA_{0.7}MA_{0.3}Pb_{0.5}Sn_{0.5}I_3$, with a bandgap of 1.22 eV, employed as the absorber layers in the top cell and bottom cell, respectively. This approach mitigates thermalization and transmission losses, resulting in improved power conversion efficiency (PCE). The proposed work demonstrates the impact of active-layer thickness and defect density on solar cell performance. Additionally, an investigation into various electron transport layers (ETLs) and hole transport layers (HTLs) has been conducted to optimize the performance of both the top and bottom cells. Using filtered-spectrum analysis and the current matching method, various performance parameters of the solar cell have been calculated. For the proposed device structure, the open-circuit voltage (Voc) is 1.57 V for the top cell and 0.92 V for the bottom cell. The short-circuit current density (Jsc) is 22.05 mA/cm² for the top cell and 34.10 mA/cm² for the bottom cell. The fill factor (FF) is 79.90% for the top cell and 83.30% for the bottom cell. The power conversion efficiency (PCE) is 20.75% for the top cell and 24.80% for the bottom cell in perovskite tandem configuration.

H1-0023

Compositional Dependence on Glass Transition Temperature in Germanium Telluride Based Glasses on The Network Connectivity

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A theoretical framework describing the viscosity increase due to agglomeration of covalant bonds in the glass network as a result of changes in the structural units is presented. The glass transition temperature as a function of network parameter in binary GeTe system is analyzed. The issue related to network entropy in modified network is also discussed.

I1- 0001

Materials for Hydrogen Energy Harvesting

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Abstract

Energy is a necessary component of human life; nevertheless, the world is facing an energy crisis due to exponential population growth and limited fossil resource availability. Because of its increasing availability, it necessitates prompt attention. Solving this energy demand with more efficient or clean alternative energy sources could not only save the planet from bad environmental effects, but it could also reduce inequities and create a more peaceful society [1]. The ability to supply high-capacity, low-cost clean energy production and storage technologies will be vital to integrating low-carbon renewable energy into national and international energy networks completely and successfully. Hydrogen is frequently seen as a safe, feasible alternative to conventional fuels. Fossil fuels, which include coal, oil, and gas, account for more than 75% of all greenhouse gas emissions and over 90% of total carbon dioxide emissions, making them the world's main cause of climate change [2]. Another element contributing to India's rapidly increasing demand for renewable energy is the country's burgeoning population. Aside from fuels, hydrogen energy is employed in a range of applications, the most notable of which is the development of efficient, cost-effective, and sustainable energy, including water-splitting electrolysis and fuel cells. Hydrogen is referred to as clean energy since when it is used, it just emits water vapour and no other byproducts into the atmosphere. Fuel cells with electrolysis that separates water improved energy conversion efficiency. On Earth, stable and abundant electro-catalysts are required to accelerate the slowing of the hydrogen-oxygen reaction. The advanced materials began by favoring electro catalysts for hydrogen and oxygen. For clean energy (hydrogen) production and storage, innovative materials, and process technologies such as hydrogen and CO_2 based energy carriers and hydrogen energy storage via phase change materials or reversible thermochemical reactions are being researched [3]. Nanomaterials, one of the most important materials today, have been proposed as sources of energy generation and storage due to their outstanding properties and ease of manufacture [4]. Nanopartials, nanotubes, 2D materials, leached quasicrystals and High Entropy alloys are some examples. It will be discussed how such functional materials can be used to use for hydrogen production and storage.

I1- 0002

Simulation Study of CTS Solar Cell Using SCAPS

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Abstract

The work reports the simulation study of the CTS solar cell using the software SCAPS. The software helps to form a hetero structure for thin film solar cell by making various combinations of materials such as absorber layer and buffer layer. Further, the graphs and results obtained can be simulated. CdS Material used as buffer layer, ZnO used as window layer. whereas CTS material is used as absorber layer. For various combinations of Buffer /Absorber material thickness, the efficiency comes out to be different, depending upon the e-h pair generated. We get the maximum efficiency w.r.t Thickness of the Absorber layer. Band alignment at the absorber/buffer interface should be proper which can be obtained by selecting the materials with appropriate values of Electron Affinity. Here by changing values of Series and Shunt resistance significance of resistance can be measured. The band gap energy of the buffer layer and absorber layer should also be compatible with each other. The ideal thickness of the buffer layer is also identified with each absorber layer which results in noticeable change in fill factor and efficiency of solar cell.

I1- 0003

Insights into Structural, Morphological and Electrochemical Improvements in Mn_3O_4 Thin Films with Borax Incorporation

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Abstract

This work investigates the synthesis of Mn_3O_4 thin films with borax incorporation using the spray pyrolysis technique. Structural analysis through X-ray diffraction (XRD) and Raman spectroscopy confirms the retention of the tetragonal Mn_3O_4 phase, with noticeable reductions in diffraction peak intensity and shifts in Raman modes indicating effective borax integration. Field emission scanning electron microscopy (FESEM) revealed significant morphological changes, showing dense wrinkles and sodium agglomerations. Further, the addition of borax has increased surface roughness and decreased the contact angle, suggesting improved surface wettability. X-ray photoelectron spectroscopy (XPS) confirmed boron incorporation at interstitial sites, along with oxygen imbalance and changes in the oxidation states of manganese. Moreover, electrochemical analysis through cyclic voltammetry (CV) and galvanostatic charge/discharge (GCD) demonstrated enhanced specific capacitance after borax incorporation. Also, a reduced charge transfer resistance in borax-incorporated films was revealed by electrochemical impedance spectroscopy. This improvement highlights the potential of borax-incorporated Mn_3O_4 thin films as promising electrode materials for supercapacitor applications.

I1- 0004

Optimizing MoO_3 Thin Films for Enhanced Photoelectrochemical Water Splitting: Influence of Substrate Temperature on Phase Formation

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Abstract

Conventional fossil fuels are non-renewable and environmentally harmful, while hydrogen (H_2), on the other hand, is gaining attention as a cleaner alternative with water as its only combustion by-product. This study explores MoO_3 thin films synthesized via spray pyrolysis technique as potential photoelectrode materials for PEC water splitting, aiming to tune the band gap for enhanced performance. Structural analysis using X-ray diffraction (XRD) and Raman spectroscopy showed that substrate temperature significantly influences MoO_3 phase formation: both α- and h-phases appear at lower temperatures (250–275°C), while a pure α-phase forms at higher temperatures (300–375°C). The α-phase is characterized by a peak along the (040) plane at 25.7°, with optimal film quality observed at 350°C. SEM analysis revealed increased compactness with increase in substrate temperature, and EDS confirmed the Mo:O stoichiometric ratio. Diffuse reflectance spectroscopy (DRS) indicated an absorption edge around 385 nm, with consistent band gap energies across temperatures. Photoluminescence spectra exhibited emissions associated with defect states. In conclusion, optimizing substrate temperature is crucial for achieving high-quality MoO_3 photoelectrodes.

I1- 0005

Enhancement of the Photoresponsiveness of Alizarine Red S in Photogalvanic Cell

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Abstract

Photogalvanic cell, a solar energy conversion device, holds promise for development of new and sustainable energy technology. It is still in research phase. Its utility increases due to the direct conversion of solar energy into electrical energy. The photogalvanic effect has been observed in Alizarine Red S – Galactose – Acacia Concinna cell system. This photosensitizer, reductant and natural surfactant combination provided enhanced photoresponse towards solar radiation. The cell function studied in alkaline (NaOH) medium with and without $Al(OH)_3$ solution in detail. The developed cell showed optimum cell parameters in terms of Photopotential, Open-Circuits Potential, Maximum Current, Short-Circuit Current and Storage Capacity ($t_{1/2}$) are 139mV, 314mV, 28µA, 6µA and 1330 minutes, respectively. In presence of natural surfactant Acacia Concinna and $Al(OH)_3$, PG system has been showed efficacious enhancements in storage capacity.

Keywords: Alizarin Red S, Galacstose, Acacia Concinna, Storage Capacity, Photogalvanic cell.

I1-0006

Electrochemical performance of polycrystalline $Dy_{2-x}Bi_xCoMnO_6$ compound as a supercapacitor electrode

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Abstract

The present work reports the electrochemical behavior of the Bi-doped double perovskite Dy_2CoMnO_6 (DCMO) compound. Polycrystalline double perovskite $Dy_{2-x}Bi_xCoMnO_6$ (x = 0, 0.4,0.8, 1.2, and 1.6) samples were synthesized using the solid-state reaction method. The prepared samples were characterized by X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), energy dispersive spectroscopy (EDS), X-ray photoelectron spectroscopy (XPS) and cyclic voltammetry (CV) techniques. Analysis of the room temperatureXRD data shows that all the samples crystallize in the monoclinic phase with the space group$P2_1/n$. The surface morphology of each sample was examined using the FE-SEM technique. FE-SEM images exhibit a homogeneous distribution of grains with tiny spaces throughout thesurfaces for all the samples. The EDS spectrum confirms that all the samples contain only thedesired elements (Dy, Bi, Co, Mn, and O) in the appropriate amounts. Results of our XPS study reveal the existence of multiple oxidation states of Co and Mn (Co^{3+}/Co^{+2} and Mn^{+3}/Mn^{4+}) within the samples. Cyclic voltammetry was employed to examine the electrochemical performance of the prepared electrode of doped and undoped DCMO compounds. Capacitance was increased at different scan rates with Bi-doping in the DCMO compound. Cyclic voltammograms (CV) and galvanostatic charging-discharging (GCD) curves of $Dy_{0.8}Bi_{1.2}CoMnO_6$ show a sizable specific capacitance with extraordinary cyclic stability. This work produces efficient and stable double perovskite oxide i.e. DCMO as a supercapacitor electrode for energy storage applications.

I1- 0007

Tin Chalcogenides: A promising Thermoelectric Series for Mid-Temperature Power Generation

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Abstract

The rising demand of sustainable and environmentally friendly energy sources has thrusted considerable research into green energy, energy storage and waste energy management. Thermoelectric materials have emerged as promising candidates due to their ability of direct conversion between heat and electricity which has great potency in power generation, waste heat recovery and Peltier effect-based heat pumping. Lead chalcogenides are mid-temperature thermoelectric materials with high ZT magnitudes but toxicity of lead has inspired the researchers to approach lead free Tin chalcogenides. This article provides a comprehensive review of recent advancements in Tin chalcogenides specifically SnTe, SnSe and SnS with prime focus on thin films and nanoparticles-based Tin chalcogenides. We firstly outline their fundamental properties and synthesis methodologies for bulk and thin film samples with synthesis parameters. The variation of electric and thermal transport character of material with synthesis techniques and their role in affecting the figure of merit and hence efficiency of thermoelectric material are discussed. The key strategies employed to enhance the efficiency of thermoelectric material by optimizing the electron and phonon transport are summarized. Towards the end of the article, we provide insights into current challenges and future research directions for scaling thermoelectric functionality of these materials for practical applications.

I1- 0008

Electrical Transport Properties of Solid Cu^{+}/Cu^{2+} Redox Mediators for Dye-Sensitized Solar Cells

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Abstract

In Gulf countries' hot weather, a solid electrolyte is required to regenerate dye molecules. The solid nature of the electrolyte keeps the dye-sensitized solar cell lightweight, unbreakable, and safer. In this article, we reported electrical transport properties of new solid Cu^{+}/Cu^{2+} redox mediators (electrolytes), utilizing ionic salts such as LiTFSI, $Cu(dmp)_2(TFSI)$, and $Cu(dmp)_2(TFSI)_2$ in a matrix of [(1-*x*)succinonitrile: *x* poly(ethylene oxide)], where $x = 0$, 0.5, and 1 in weight fraction. The electrolyte with $x = 0$ was synthesized by heating the ingredients at 65 °C and stirring for 24 h, which is similar to that of the liquid electrolyte by Saygili et al. (#A: 0.1M LiTFSI, 0.2M $Cu(dmp)_2(TFSI)$, and 0.04M $Cu(dmp)_2(TFSI)_2$ in acetonitrile) and Mathew et al. (#B: 0.1M LiTFSI, 0.25M $Cu(dmp)_2(TFSI)$, and 0.06M $Cu(dmp)_2(TFSI)_2$ in acetonitrile). We prepared the poly(ethylene oxide)-based electrolytes ($x = 0.5$ and 1) by the solution cast method. The liquid electrolytes exhibited electrical conductivity ($\sigma_{25°C}$) values: 1.6×10^{-3} (#A) and 2×10^{-3} S cm^{-1} (#B). The electrolytes ($x = 0$) observed $\sigma_{25°C} \approx 2.2\times10^{-5}$ (#A) and 2×10^{-4} S cm^{-1} (#B). The electrolytes with $x = 1$ achieved $\sigma_{25°C} \approx 2.6\times10^{-7}$ (#A) and 1.54×10^{-7} S cm^{-1} (#B). The electrolytes with $x = 0.5$ had $\sigma_{25°C}$ of 4.4×10^{-4} (#A) and 2.4×10^{-4} S cm^{-1} (#B). The log σ–T^{-1} study exhibited Arrhenius-type behavior for liquid and solid electrolytes ($x = 0$ and 1) and Vogel−Tamman−Fulcher-type behavior for the electrolytes with $x = 0.5$. Various studies using XRD, FT-IR spectroscopy, DSC, and TGA shed light on the electrical transport properties.

I1- 0009

Analyzing Pseudo-capacitive behaviour of Co-doped MoS_2 on a Screen-Printed Carbon Electrode

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Abstract

Energy harnessing and storage are urgent needs of the present, and supercapacitors offer as one of the most promising technologies in the future. Transition metal (TM) doping is an effective method to enhance the electrochemical activity of MoS_2 by improving its conductivity and introducing additional redox sites through the dopant atoms. This work used a hydrothermal technique to concurrently synthesize Co-doped MoS_2 with increased pseudocapacitive properties on screen-printed carbon electrodes. The morphological characterization was performed using X-ray diffraction (XRD) and Scanning electron microscopy (SEM). Electrochemical analysis was done by cyclic voltammetry (CV) in a potential range of -1.5 V to 1 V at a scan rate of 10 mV/s, 20 mV/s, 40 mV/s, 60 mV/s, 80 mV/s, 100 mV/s, 200 mV/s, 400 mV/s, 600 mV/s, 800 mV/s, 1 V/s. The CV profile shows good stability and reversibility even at high scan rates with a proper pseudo-capacitive behaviour. The areal capacitance calculated at 10 mV/s is 7.56 F/cm^2 . Electrochemical impedance spectroscopy (EIS) analysis (from 1Hz to 50 kHz) also endorses pseudo-capacitive behaviour of the synthesized materials. Thus, Co-doped MoS_2 is a promising candidate for electrode material.

I1- 0010

Silicon and its Composites as Anode Materials in Li-ion Batteries

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Abstract

Recent technological advances need a reliable and sustainable energy storage system with a high energy density. Current Li-ion batteries use LiCoO2 and graphite as cathode and anode materials respectively, but have limited capacity. The anode side of the battery plays important function in storing Li-ions during charging and discharging cycles. Si has evolved as a unique anode material in recent decades with a theoretical capacity almost ten times that of traditional graphite. But, there are various issues with Si, like massive volume expansion, electrode pulverization, decreasing cell capacity over time, etc. The electrochemical performance of Si and its composites determined by the materials utilized. Direct alloying of Si with Li yields stable phases such as Li12Si7, Li7Si3, Li13Si4 and Li21Si5 with the highest theoretical capacity. Composites of Si, which include carbon, polymer and other elements, exhibit promising outcomes. This paper summarizes and discusses current breakthroughs in Si and its composites tested as anodes in Li-ion batteries. The use of 1D, 2D and 3D carbon with various matrices for Si composite helps to accommodate volume expansion. Structural and morphological changes as well as the electrochemical performance of thus synthesized batteries have also been described.

I1- 0011

A Review on Importance of Rate of cooling of Gas hydrates in clay environments with non-stirred reactor

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Abstract

We experimented with gas hydrate in various clay media. We discovered that in a clay environment, the rates of methane conversion were evidently smaller for higher Rw ratios than those in other media experimentally. We express that it is because of the distinct water compositions at various pressures in different media that caused the differences in induction time and rate of cooling. In sediments like clay, because of its Due to the small particle size, the proportion of bound water is much higher than in sand, and the bound water is more difficult to hydrate.During thawing cycles, our experiments shows that the rate of formation after sub-cooling temperature has rapid growth during the saturation level.

I1- 0012

Pulsed Laser deposited FeSi thin films: Effect of sulfurization on structural and optical properties

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Abstract

Fe2SiS4 is one of the earth-abundant light-absorbing semiconductors and is thermodynamically stable compound of pyrite FeS2. In the present study, initially we have prepared Fe-Si target for pulsed laser deposition. The target is prepared by step melting of elemental Fe and Si inside a vacuum evacuated and sealed ampoule followed by quick quenching. On x-ray diffraction study, it has been found that the target is consisting of Fe5Si3 phase having hexagonal structure. By ablating prepared Fe5Si3 target by pulsed laser, thin film are deposited on soda lime glass by varying energy flux, pulse frequency of incident laser and substrate temperature. The deposited thin films are found to exhibit of similar crystal structure as noticed in the target. The prepared FeSi thin films are converted to corresponding sulphur phase by annealing in sulphur ambient in the temperature range 300-500ºC. After sulfurization changes in microstructure are seen by scanning electron microscopy. Optical band gap is found in the range 1.25-2.75 eV depending upon deposition and sulfurization conditions. Electrical conductivity measurements in the temperature range 50-300 K were also done indicating semiconducting nature of the sulfurized FeSi thin films.

Keywords: Pulsed laser deposition, FeSi, thin films, post-deposition sulfurization

I1- 0013

NASICON: A Comprehensive Review of Structure, Properties, and Applications in Sodium-Ion Batteries

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Abstract

Sodium Super Ionic Conductor, or NASICON, materials have shown great promise as solid electrolyte alternatives for sodium-ion batteries because of their high ionic conductivity, structural stability, and adaptability. With an emphasis on their crystal structure, electrochemical characteristics, and the variables influencing their performance in sodium-ion battery applications, this article offers a thorough analysis of materials of the NASICON type. We examine several synthesis techniques, ionic conductivity enhancing changes, and electrode interface compatibility procedures. Furthermore, future possibilities in research aiming at overcoming these limitations are highlighted, as well as the difficulties associated with scaling up NASICON materials for commercial use. An in-depth analysis of NASICON's contributions to developing sodium-ion battery technology and its potential for large-scale electricity.

Keywords: NASICON, sodium superionic conductor, solid electrolytes, sodium-ion batteries, ionic conductivity, structural stability, crystal structure, electrochemical performance, synthesis techniques, electrode interface compatibility, scalability, commercial applications, energy storage, large-scale electricity.

I1- 0014

Optimizing Mn-Doped V_2O_5 for Superior Performance in Photocatalytic and Energy Storage Systems

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Abstract

The primary global issues of the 21st century is freshwater scarcity, pollution from industrial dyes, and the development of efficient energy storage devices. Over 700,000 tons of synthetic dyes are produced annually, with more than 15% ending up in water bodies. Additionally, advancements in energy storage devices are crucial for mitigating the environmental impact of energy consumption and transitioning towards sustainable energy sources. In this perspective, vanadium pentoxide (V_2O_5) has attracted considerable attention as a photocatalyst and a cathode material for energy storage devices due to its outstanding properties such as low cost, narrow bandgap (~2.3 eV), optical and chemical stability, and multiple oxidation states. Furthermore, in recent years, biological synthesis has emerged as an attractive alternative to traditional chemical and physical methods for producing nanomaterials. However, the narrow band gap of V_2O_5 also makes it easier for the photogenerated electrons and holes to recombine in the excited state, and the stored energy is instantly consumed by carrier recombination which affects the photocatalytic and cyclic stability for energy storage devices. Therefore, promoting the carrier separation of V_2O_5, improving the photocatalytic efficiency, and increasing the cyclic stability are the key problems to be solved. Several methods to improve the photocatalytic performance and electrochemical performance of V_2O_5 including metallic ion doping, non-metallic ion doping, semiconductor recombination, and noble metal deposition are reported to enhance its performance. In the present study, we have synthesized the pure and Mn 4% doped V_2O_5 using a solid-state reaction method. XRD, SEM, TEM, and EDS characterized the prepared samples. Further, the effect of Mn doping on the solar-driven photocatalytic efficiency of the V_2O_5 was tested against the methylene blue dye under solar irradiation. The electrochemical performance of prepared samples as a cathode material for Li-ion batteries was tested using a three-electrode system with $LiPF_6$ as an electrolyte.

I1- 0015

Photophysical Analysis of the Surfactant System for Solar Energy Storage and Conversion in Photogalvanic Cells

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Abstract

The most important component of human society that enters into progressive processes is energy. Any nation's only means of survival in terms of progress and security is through its access to energy. Solar energy is directly converted into electrical energy and stored using photogalvanic cells. The foundation of photogalvanic cells is the photochemical reaction that, upon activation by a photon, yields high energy products. These energy-dense compounds lose electrochemical energy, which causes the creation of electricity. For better electrical results, the specially constructed H shaped Photogalvanic (PG) cells were studied. We used a spectrometer, a digital pH metre, a resistance key, a carbon pot, and a micro-ammeter. In a PG cell system, the various solar parameters were investigated. By changing the various parameters of the PG cell, the most significant impact of solar energy has been studied. Both the photopotential and the photocurrent were measured to be 697 mV and 290 μA, respectively. Performance and conversion efficiency for the PG cell have been found to be 123.00 minutes and 0.2749%, respectively. The best and alternative energy source to help meet the world's energy needs is solar energy. For the current generation of PG cells, a suggested photochemical mechanism for the transformation of solar radiation energy was provided. The main goal of the research was to increase meaningful electrical output. By detecting the positive number of electrical outcomes in the PG cell system, the objective has been accomplished. Possibilities exist to improve the conversion and storage of solar energy using photogalvanic cells by choosing an appropriate photosensitizer and reluctant in addition to having a wider range of combinations of two distinct surfactants. Cell photogeneration is facilitated through a photochemical mechanism.

I1- 0016

A physical interpretation for variation of lifetime with level of injection in amorphous semiconductors

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Abstract

An analysis of variations in lifetime of amorphous semiconductors is presented in terms of excitation level defined by separation of quasi-Fermi levels of electrons and holes. A transition from dangling bond dominated region to tail states dominated region is found to occur in terms of level of excitation. Based on the recombination statistics for correlated dangling bond states, a peak in the lifetime of excess carriers is obtained at the transition. Below the transition the lifetime increases with increasing generation rate of electron-hole pairs whereas above it there is a decrease in the lifetime. Presence of other impurities moves the position of this transition. Also, inclusion of recombination via tail state may reduce the increasing trend in the lifetime below the transition but reduction in the lifetime at higher level is still observed.

I1- 0017

The Electrocatalytic study of Low-cost, Sustainable Biowaste-Derived Carbon-Metal Composite in varying Alkaline pH Electrolytes for Efficient Hydrogen Evolution Reaction

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Abstract

The degradation of fossil fuel due to its excess use has led the world to search for an alternative source of energy that is abundant, cheap, and environmentally friendly. Herein, we report the electrocatalytic survey of easily available, cost-effective, and biomass-derived carbon-metal composite synthesized at 750^0C using cobalt (Co) and molybdenum (Mo) precursors for Hydrogen evolution reaction (HER) in alkaline electrolytes with different pH. The physical characterizations (like XRD, RAMAN, FE-SEM) confirm the formation of nanoporous graphite-like carbon-metal composite (CCoMoO@750^0C). The electrochemical characterization reveals the effect of different alkaline pH (9.5, 11.2, and 12.6) on the electrocatalytic HER activity of CCoMoO@750^0C. For HER, the as-synthesized catalyst requires a low overpotential of about -0.250V to achieve the benchmark current density of -10mA/cm^2 in an electrolyte with pH 12.6, -0.274V at -10mA/cm^2 (in pH 11.2), and -0.291V at -10mA/cm^2 (in pH 9.5).

I1- 0018

Oxidation Kinetics studies of $Ti_3C_2T_x$ MXene using Freeman-Carrol method

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Abstract

$Ti_3C_2T_x$ MXene is synthesized from $Ti_3AL_2C_3$ MAX phase by using HF treatment and characterized by x-ray diffraction and infrared spectroscopy. In addition, Oxidation of $Ti_3C_2T_x$ MXene in nitrogen environment from room temperature to 500-degree Celsius is studied by thermogravimetric analysis. Experiments shows that oxidation of $Ti_3C_2T_x$ MXene starts at 275 degree Celsius. Activation energy of oxidation of $Ti_3C_2T_x$ MXene is estimated using Freeman Carrol method based on Arrhenius equation. It is shown that in nitrogen environment and in strong oxidation temperature range, oxidation activation energy of $Ti_3C_2T_x$ MXene is in kJ mol^{-1}.

I1- 0019

Dimensionally Stable Nickel Iron selenide/oxyhydroxide Catalysts for Water and Urea Electrolysis for Industrial Scale hydrogen production

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Abstract

Rational design and optimized electrodes structure have huge impact on elevating the catalytic performance for water and urea electrolysis for hydrogen generation. In the present research, nickel iron selenide/hydroxide composite ($Ni_xFe_3Se_4$-OOH) catalysts have been facilely deposited on nickel foam using chemical bath deposition which can be expanded to industrial scale large area electrode fabrication without using polymeric binders. Fe_3Se_4-OOH catalysts, having low interfacial resistance and abundance of catalytically active sites, shows excellent electrocatalytic performance, requiring overpotential of 174 mV at 10 mA/cm^2 for hydrogen evolution reaction (HER) and 243 mV (1.47 V vs RHE) at 20 mA/cm^2 for oxygen evolution reaction (OER). Further, the Fe_3Se_4-OOH catalysts on nickel foam exhibits the efficient urea oxidation due to abundance of NiFe oxyhydroxide and generates the geometric current density of 20 mA/cm^2 at anodic potential of 1.36 V vs RHE, lowering the potential requirement by 110 mV due to thermodynamically favourable reaction mechanism. Bi-functional water and urea electrolyser using $Ni_xFe_3Se_4$-OOH catalysts shows excellent performance, requiring the cell voltage of 1.71 V to generate 100 mA/cm^2 current in laboratory conditions (1M KOH, 25°C), while the cell voltage is reduced to 1.58 V (at 100 mA/cm^2) in industrial condition (5M KOH, 60°C) and also exhibiting excellent stability at industrial scale current of 300 and 1000 mA/cm^2 for 50 hours. For urea electrolysis, cell voltage is about 1.67 V in 1M KOH + 0.33 M urea and 1.65 V in 5M KOH + 0.33 M urea to generate 100 mA/cm^2.

Keyword: Industrial scale hydrogen production; water splitting; urea oxidation; chemical bath deposition.

I1- 0020

Camphene - Fatty Alcohol - based Eutectic Phase Change Materials for Thermal Energy Storage Applications

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Abstract

Despite extensive research on phase change materials (PCMs), most studies rely on experimental trial-and-error methods to test component combinations for eutectic PCMs, which are costly, time-consuming and inefficient for systematically discovering new eutectics when screening large numbers of candidate materials. In this study, the thermophysical properties of novel eutectic PCMs composed of camphene and various fatty alcohols, including 1-dodecanol, 1-tetradecanol, 1-hexadecanol and 1-octadecanol, were theoretically calculated using the thermodynamical principles based on solid-liquid equilibria. The eutectic mixtures have eutectic compositions ranging from 26-71 mol% camphene, with melting temperatures between 17.55 °C to 40.76 °C and latent heats of fusion varying from 211-234 J/g. These theoretical studies offer an efficient and cost-effective alternative to experimental screening. They provide valuable insights into the thermophysical properties of camphene-fatty alcohol-based eutectic PCMs, potentially expanding their applications in thermal energy storage systems, such as building heating and cooling.

Key Words: phase change material, eutectic, theoretical, melting temperature, thermal energy storage

I1- 0021

Electronic Characteristics of Multinary Chalcogenide Semiconductors for Energy Applications

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Abstract

In the field of energy applications, particularly in thin-film solar cell technology, multinary chalcogenide semiconductors are of significant interest due to their tunable and favorable optoelectronic properties. The multinary compound $CuZn_2AlS_xSe_{4-x}$ represents a vital area of research, offering unique characteristics that can be harnessed for next-generation electronic and optoelectronic applications. In this study, we utilized density functional theory through the Wien2k code to investigate the electronic properties of $CuZn_2AlS_xSe_{4-x}$ materials. The density of states and band structure were calculated using the Perdew-Burke-Ernzerhof (PBE) functional. Our findings indicate that this compound behaves as a direct band gap semiconductor, with transitions occurring at the gamma point between the valence and conduction bands. The bandgap decreases when sulfur (S) anions are replaced with selenium (Se), however, the overall band characteristics remain consistent for both S and Se. This compositional tunability significantly enhances light absorption and charge carrier mobility, which are critical factors for improving energy application efficiency.

I1- 0022

PVDF -HFP/WS_2 based triboelectric nanogenerator for harvesting the mechanical energy from human motion

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Abstract

Energy harvesting from ambient energy sources and human motion is a viable strategy for self-powered wearable and portable electronics. Triboelectric nanogenerators (TENGs), a novel emergent technology, have received a lot of interest for its ability to capture mechanical energy from the environment and transform it into electricity. Here, we have developed a high performance triboelectric nanogenerator by coupling of PVDF -HFP/WS_2 nanocomposite film with PDMS film as two triboelectric layer for TENG fabrication. To do this, different weight percentage of WS_2 nanosheets are incorporated in the PVDF -HFP matrix and, the resulting thin films are structurally and morphologically analyzed using XRD, FTIR, and SEM techniques. The results show that adding WS_2 nanosheets to a PVDF matrix improves the triboelectric characteristics of PVDF-HFP films due to their large surface area and excellent electron affinity. Finally, the fabricated nanogenerator is utilized to harvest the mechanical energy from human motions, such as, finger tapping, foot tapping, elbow bending etc. Thus, the current study provides a versatile, cost-effective, and environmentally friendly approach for harvesting biomechanical energy from human motions, enabling a wide range of applications from portable electronics to wearable devices.

I1- 0023

Graphitic-Carbon Nitride Embedded PVDF-HFP Film for Enhanced Performance of Piezoelectric Nanogenerator

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Abstract

With advancements in wearable electronic devices, the demand for flexible, efficient, and sustainable energy sources is rapidly growing. Until now, energy requirement of these portable devices are fulfilled by the batteries, but they have a limited lifespan. In this context, piezoelectric nanogenerators offer a promising solution for developing self-powered sustainable system by harvesting the mechanical energy from the living environment. In this study, we synthesized graphitic carbon nitride (g-C_3N_4) using a one-step pyrolysis method and incorporated it into PVDF-HFP by varying the weight percentage of g-C_3N_4 to prepare polymer nanocomposite films for fabricating piezoelectric nanogenerators. The prepared powder samples and films were characterized for their structural and morphological properties, and their piezoelectric response was evaluated using a dynamic shaker. The results demonstrate that the addition of graphitic carbon nitride significantly enhances the output performance of the PVDF-based piezoelectric nanogenerator, highlighting its potential application in wearable electronic devices.

I1- 0024

Electrode-Electrolyte Interface Engineering in Lithium-based Batteries: Towards Sustainable Energy Solutions

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Abstract

The advancement of lithium-based rechargeable batteries, (i.e., Li-ion, Li-S, and Li-metal), plays a pivotal role in enabling a sustainable energy future and meeting the increasing demand for high-energy storage solutions. This work presents recent innovations in battery technology, emphasizing breakthroughs in electrode and electrolyte engineering to improve performance, safety, and cost-effectiveness. Special attention is given to lithium metal batteries, highlighting their potential to revolutionize the energy storage landscape. By addressing key challenges such as battery electrode synthesis, electrolyte formulation, and overall battery design, this study demonstrates the transformative impact of these advancements on the development of next-generation batteries. The findings underscore opportunities for practical applications, offering insights into how these innovations can drive progress in the industrial sector and contribute to more efficient and safer energy storage solutions.

I2- 0001

Electronic structure and optical properties of quaternary Heusler compound LiTiRhGe: first principles study

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Abstract

In current study the electronic structure and optical properties of quaternary Heusler compound LiTiRhGe have been investigated through first-principles calculations using the GGA-PBE approximation implemented in Wien2k within density functional theory. In the study we found that the compound is indirect band gap semiconductor in nature. Density functional theory is again used to investigate the optical properties of materials such complex dielectric function, optical conductivity, refractive index, and reflectivity. Considering the lack of previous research on optical properties of LiTiRhGe, this study provides a vital reference for thorough analysis of this compound, opening the door for theoretical and experimental studies in this area.

Keywords: Band structure, optical properties, density functional theory, quaternary Heusler compound.

I2- 0002

Fabrication of Crystalline Silicon Solar Cells With Transition Metal Oxide Heterocontact as More Economical and Eco-Friendly

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Abstract

Population expansion, industrial growth, and a range of industries are all contributing to increased global electricity demand. Fossil fuels, including coal, oil, and natural gas, produce insufficient electricity and are depleting due to extraction. Non-traditional energy sources, including solar, wind, and biomass, have the ability to meet world electricity needs. Photovoltaic technology is essential for a sustainable global energy supply. Solar cells are efficient, with a lifespan of more than 20 years, and offers environmental advantages. Photovoltaic technology, which converts solar energy into electricity, has an efficiency of around 25%, and silicon heterojunction technology (SHJ) achieves a high efficiency of 26.7% with doped a-Si:H heterocontact; however, they emit poisonous and combustible fumes, use complex deposition methods that harm the environment, and have energy losses such as parasitic and Auger recombination, which necessitate special safety precautions and are expensive. Transition metal oxides (TMO) can be utilized as an alternative to doped a-Si:H heterocontact since they are readily accessible, inexpensive, and non-toxic, as well as easily depositionable utilizing a simpler technique at temperatures below 200 °C. This study created a c-Si solar cell using TMO's titanium dioxide and molybdenum trioxide as electron and hole selective contacts, respectively, and SiO2 as a passivation layer. The c-Si solar cell had an efficiency of around 24.75%, which boosted its performance and increased its potential to more than 28.4%. TMO's heterocontact solar cells have the potential to be cost-effective and highly efficient for large-scale industrial manufacturing, as well as environmentally friendly and providing society with a levelized cost of electricity.

I2- 0003

Crystal Growth and Structural Characterization of $Bi_{0.95}Sb_{0.05}$ Topological Single Crystal

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Abstract

We report the growth and structural characterization of $Bi_{0.95}Sb_{0.05}$ topological insulator. $Bi_{0.95}Sb_{0.05}$ single crystal was synthesized by melting bismuth and antimony together using the facile self-flux method via solid state reaction route in an automated programmable tube furnace. The on surface X-ray diffraction (XRD) pattern on as grown crystal flake displayed 00l alignment and revealed the crystalline nature of the resultant $Bi_{0.95}Sb_{0.05}$ crystal. Rietveld refinement of powder XRD data confirmed the phase purity and rhombohedral crystal structure with R-3m space group. Further, the unit cell structure formed using the VESTA software verified the rhombohedral crystal structure. Scanning electron microscope (SEM) and energy dispersive X-ray analysis (EDXA) mapping images taken on freshly cleaved $Bi_{0.95}Sb_{0.05}$ single crystal flake displayed the layered directional growth with homogeneous distribution of Bi and Sb elements. Elemental mapping of the resultant $Bi_{0.95}Sb_{0.05}$ single crystal showed that the constituent elements (Bi and Sb) are homogeneously distributed in accordance to their stoichiometric ratio.

I2- 0004

Induction of Room Temperature Ferroelectric Phase In a Multi-component Liquid Crystal Mixture Suitable For Display Application

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Abstract

Ferroelectric liquid crystals (FLC) can be promising in display application for their high speed in-plane switching. Most FLCs exhibit ferroelectric behaviour at higher temperature. Thus there had been constant effort to formulate ferroelectric liquid crystal mixtures, with ferroelectric SmC* phase in room temperature. We had successfully formulated a FLC mixture which showed mesophases in room temperature by doping a chiral fluorinated ferroelectric liquid crystal into an achiral pyrimidine based host mixture having smectic C phase (details of this host is published elsewhere [1]).

The phase behavior, structural and elctro-optical properties of the newly formulated mixture were characterized by optical polarizing microscopy (OPM), Synchrotron diffraction studies and frequency dependent dielectric relaxation study. The spontaneous polarization, electrical response time and rotational viscosity were also measured. The mixture was found to exhibit ferroelectric SmC* phase below room temperature (less than 15ºC) and the phase is found to exist over a wide temperature range. It also shows SmA* phase before melting into isotropic phase. Further, the SmA* phase is found to exhibit partial de Vries type property and electroclinic effect. In the low temperature region of SmC* phase the layer spacing of the mixture is in between the host and the dopant while the tilt is found to be much higher in the mixture than in the host and the dopant. It was found to have moderate spontaneous polarization. Optical tilt of around 20° at room temperature and a response time of a few hundred microseconds make the mixture suitable to use in SSFLCDs.

I2- 0005

Impact on the Dielectric and Raman spectroscopic properties of the nematic liquid crystals with the function frequency and temperature

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Abstract

In the present study, we investigate the dielectric and Raman spectroscopic properties of the liquid crystal compound 1, 12-bis (4-(E-naphthalen-2 yldiazenyl) phenoxy) dodecane (C44H46N4O2) with the function of the temperature. Dielectric permittivity and loss-tangent (Tan δ) are determined by the measurement of the phase impedance analyzer with the function of temperature and frequency. Dielectric permittivity and tan δ are determined by the measurement of the phase impedance analyser with the variation of temperature and frequency. Relaxation frequency increases with the increase in temperature and is optimized at a certain temperature of the liquid crystal compound. Tan delta and dielectric permittivity are associated with the combined effect of the molecular polarizability of LC molecules with the applied electric field. The dispersive nature of the LC compound temperature dependence on their characteristic relaxation frequency reveals the existence of relaxation behaviour, which exhibits the Cole-Cole and Debey theory. The phase sequence of the liquid crystal compound has been verified by the DSC (Differential Scanning Calorimetry) graph and optical texture with the respect to temperature. Raman spectra have been analysed to better understand their molecular interaction, phase transition, and orientational order parameters for display and photonics applications. For analysing the vibrational mode of the LC molecule's characteristics, the Raman band associated with the molecular alignment and conformational changes of the liquid crystal compound undergoes phase transitions. Our result explained that the dielectric and Raman spectroscopic properties are sensitive to structural changes induced by the temperature and applied electric field in a planar geometrical arrangement of the sample cell. Results have been explained on the spectral features, such as shift in Raman peaks and intensity changes, and how these correlate with the physical properties of the liquid crystal compound. The remarkable results provide the most understanding of the behaviour of the liquid crystal compound and their potential for tailored material design in advanced liquid crystal-based technology.

I2- 0006

Understanding the Mechanism of Hg2+ Binding with Pyridine-End Functionalized OFETs Using the Hill Equation

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Abstract

In this study, we explore the integration of a functional sensing layer atop pentacene in organic field-effect transistors (OFETs) for mercury ion detection. By applying the Hill equation, a well-established model in biochemistry, we quantitatively analyze the binding interactions between mercury ions and the Pyridine-end oligo p-Phenylenevinylenes (POPVs) sensing molecules within the channel region of the OFETs. These interactions induce significant changes in the current-voltage characteristics of the devices, directly impacting their electrical performance. The saturation current serves as a reliable indicator of mercury binding events, enabling real-time detection and monitoring.
Through the Hill equation analysis, we gain insights into the binding dynamics, with the Hill coefficient providing key information about the cooperativity of the binding process. This approach not only highlights the potential of OFET-based sensors for selective and sensitive mercury ion detection but also demonstrates the effectiveness of adapting biochemistry models to organic electronic devices. The results suggest the feasibility of using OFETs for practical environmental sensing applications, offering a novel pathway for the development of efficient, low-cost sensors for heavy metal contamination monitoring.

I2- 0007

Temperature Dependent Modulation of Textures and Switching Voltage in Cholesteric Liquid Crystals for Application in Optical and Sensor Devices

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Abstract

The cholesteric liquid crystal (CLC) mixtures known for their stabilizing property in the planar (P) and focal conic (FC) states are widely used in optical shutters and sensor devices. The temperature dependent pitch of the CLC mixtures directly affects the performance and sensitivity of CLC cells, impacting their different practical applications. In this work, the CLC mixtures were prepared using nematic liquid crystal (NLC) with 4.0 and 5.0 wt% of chiral dopant (R1011) to observe the effect of temperature on their textural and electro-optical behavior. The measurements were taken at 25, 30, 35, 40, and 45 °C temperatures using the polarized optical microscope (POM), temperature controller and electro-optical setup. Textural changes under an applied electric field showed the initial rotation of the helical axis in FC state and gradual unwinding of the helices in homeotropic state. Further, as the temperature increases, these changes occur at lower voltages because the reduced viscosity and pitch make it easier for the electric field to overcome the molecular interactions that maintain the helical structure. The electro-optical results for both CLC mixtures showed a decrease in initial transmittance with temperature, making the FC state denser and resulted in reduced switching voltage. At 50 °C, the switching voltage was found decreased from 46 V (at 25°C) to 38 V and 59 V (at 25°C) to 48 V for 4.0 and 5.0 wt% chiral doped CLC mixtures, respectively. However, the better contrast was found at 40°C and 45 °C for 4.0 and 5.0 wt% samples, respectively.

I2- 0008

Investigation of Structural Changes in Bismuth Substituted SrFe12O19 Compound Using In-Situ Raman Spectroscopy

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Abstract

The sol-gel auto-combustion method has been adopted for the preparation of bismuth (Bi) substituted strontium hexaferrite (SrFe12O19) polycrystalline compound. The substitution of bismuth has created significant distortion at various sites, which has been confirmed by the Raman spectra of Sr1-xBixFe12O19 (x = 0, 0.01, and 0.02). The compound SBFO1 (x = 0.01) is the highly strained out of three compounds. Again, the 2b and 12k site of SBFO1 is so much distorted that, the Raman peak associated to 12k site (i.e. 417.7 cm-1) has been split into two peaks at 413.8 cm-1 and 432.9 cm-1. The damping constant and spring constant calculated from the Raman data for validates the XRD data. The highest compressive volumetric strain nature of SBFO1 is well established by the lowest damping constant of SBFO1. The variation of the bond length associated to the different crystallographic sites well matches with the shifting of Raman peaks for that site. The same is again approved by the highest spring constant of SBFO1.

I2- 0009

An Effective Supramolecular Mg(II)-Metallohydrogel Based Non-Volatile Memory Device With Supreme Endurance

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Abstract

Supramolecular gels are versatile materials that possess "smart" properties. They are used in various industries such as sensors, cosmetics, foods, nanoelectronics, logic gates and regenerative medicine. These gels are formed through the combination of hydrogels and supramolecular chemistry[1]. In this work, we have developed a well-organized and efficient method to rapidly synthesize a supramolecular metallohydrogel of Mg(II)-ion which is Mg@3AP. This metallohydrogel is prepared by using 3-amino-1-pentanol as a low molecular weight gelator in water at room temperature. Here, we have investigated the hierarchical microstructural features of Mg@3AP using Field-emission scanning electron microscopy. We have analysed the metallohydrogel formation approach using FT-IR spectroscopic studies. Furthermore, we have fabricated a (Mg@3AP)-based Schottky diode device in a lateral metal-semiconductor-metal geometry to explore its charge transport behavior[2]. Here, Mg@3AP metallogel based RRAM (Resistive random access memory) device have showed a proper bipolar resistive switching behavior at room temperature. This RRAM device demonstrated exceptional switching endurance with over 10000 consecutive switching cycles and a high ON/OFF ratio of approximately 100. Due to its simple fabrication process, robust resistive switching behavior and enhanced stability, these structures are suited for applications in non-volatile memory design, neuromorphic computing.

Keywords: Mg(II)-metallohydrogel, Resistive switching, Non volatile memory, Endurance, Neuromorphic computing

I2- 0010

Effect of Na_2O/K_2O weight ratios on crystallization kinetics, conductivity and dielectric properties of niobiosilicate glasses

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Abstract

Glasses of composition SiO_2-(1-x)Na_2O-xK_2O-Nb_2O_5 (mol%) (x = 0, 1.87, 3.87, 7.5) have been synthesized through conventional melt-casting technique. A reduction in the value of crystallization peak temperature (T_p) along with increase in the peak area was observed at higher Na_2O/K_2O ratio (x = 1.87) compared to the undoped glass (x = 0). The results obtained from non-isothermal crystallization kinetics of the DSC thermograms using the Jhonson-Mehl-Avrami-Kolmogorov (JMAK) theory indicated bulk nucleation and crystal growth in the glasses. T_p area was observed to reduce and broaden with increase in K_2O content that confirmed an increase in the glass thermal stability factor against devitrification. This was corroborated with decrease in the dc ionic conductivity and increase in the activation energy of conduction (E_σ) (0.28-0.49 eVK^{-1}) of the glasses with decrease in Na_2O/K_2O ratio. The reciprocal temperature dependence of hopping frequency (ω_c) of ions for all the glasses followed an Arrhenius relation with values of activation energy (E_c) very close to E_σ signifying a common conduction mechanism for both dc and ac conduction. Scaling of real part of the complex conductivity spectra measured in the frequency range of 10 Hz to 8 MHz and in the temperature range of 498-773 K showed the curves were not perfectly superimposed which revealed a composition and temperature dependent ion conduction mechanism in the glasses. The dielectric spectra have been analyzed and correlated with the structural analysis of the effects of ions Na^+, K^+ and [NbO_6] units on the conductivity and dielectric properties of the glasses.

I2- 0011

Mesoporous Aluminum Metal-Organic Framework from Waste Alumina Dross to High Value Product for Supercapacitor Application: A Waste to Wealth Approach

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Abstract

Metal-organic framework (MOF) with high specific surface area, tunable pore size, conducting and stable structure provides a robust platform for supercapacitor applications. Herein, aluminum-based MOF (Al-MOF) has been prepared from the waste scrap alumina i.e. alumina dross using a surfactant-free soft chemical route. Alumina dross is an industrial waste that inflicts severe environmental consequences. Therefore, a mere attempt has been made to recycle the waste into a value-added product using a low-temperature scalable process. The structural analysis confirmed the phase formation. The nitrogen absorption-desorption isotherm has confirmed the presence of mesopores in the structure. Further, from the electrochemical measurement, a specific capacitance of 256 F/g @ 2 A/g has been estimated using the as-synthesized Al-MOF powder as the electrode.

Keywords: Waste; aluminum dross; Al-MOF; mesoporous; specific capacitance; supercapacitor

I2- 0012

A Simple Study of Photofieled Emission from The Bulk of A Solid

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Abstract

Photofield emission is a technique in which electron emission takes place due to joint effect of incident photon field radiation and the applied static high electric field. Due to this, the electrons emitted from the Fermi level or above it get accelerated into the vacuum regions and thus contribute to the type of emission known as Photofield emission. These emissions are constituting the electron emissions and hence contribute to the measurable current known as photofield emission current (PFEC). Several methods and techniques have been used for studying such emissions both theoretically and experimentally. For example, Gao and Reifenberger (1987) have studied the detail experimental method of photofield emission from tungsten. They have given the experimental interpretations in terms of band structures. In likewise manner, Radon and Jaskolka (1990) have studied photofield emission spectroscopy in tungsten (100) surface from Fermi level. Thapa *et. al*. have also shown the results of calculations of PFEC from tungsten by using Kronig-Penney (KP) potential method.

In this paper, we will present the application of Kronig-Penney potential models to solids like silicon which is a semiconductor. Results obtained will be compared with the earlier results that were published in CMDays-2024 Conferences, Tezpur University. The difference in the results is that earlier we have used the experimental data of dielectric constants for calculating the PFEC. In present case, the real and imaginary parts of dielectric constants of silicon were calculated theoretically by using the FP-LAPW method of density functional theory. These theoretical data will be used for calculating the PFEC and will be compared with earlier results.

I2- 0013

Effect of Silica Nanoparticles on Polymer Dispersed Liquid Crystal and Its Analysis for Smart Windows

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Abstract

Polymer-dispersed liquid crystals (PDLCs) are the materials comprised of liquid crystal (LC) droplets dispersed within a polymer matrix, and are extensively employed in modern electro-optical (E-O) applications. This study explores the comparison of morphological and E-O properties of PDLC and 0.8 wt% of silica (SiO_2) nanoparticles (NPs) dispersed PDLC cured at 0.15mW/cm^2 UV light intensity. The morphological study of the samples was performed using Polarized Optical Microscope (POM), the average droplet size was increased from ~2.5 µm to ~4.6 µm with the dispersion of 0.8wt% SiO_2 in PDLC. In E-O study, the reduction of threshold voltage (V_{th}) from 8.36V to 4.59V in 0.8wt% SiO_2 dispersed PDLC was observed as compared with pure PDLC, due to the bigger droplet sizes. In addition, a significant decrease in the operating voltage (V_{op}) of PDLC from 15.11 V to 12.49V was achieved in 0.8wt% SiO_2 dispersed PDLC. Further, the maximum transmittance (T_{max}) value was found slightly increased in SiO_2 dispersed PDLC. Moreover, 0.8 wt% of SiO_2 NPs dispersed PDLC showed higher contrast ratio (14.12) as compare to pure PDLC (7.2). The improved results observed in 0.8wt% of SiO_2 NPs dispersed PDLC are substantially correlated with the uniformity of increased droplets' size. Thus, the primed PDLCs show up a prospective relevance with the sustainable energy efficient smart windows.

Keywords: Polymer-dispersed liquid crystal (PDLC), Nanoparticles, Electro-optical, Contrast ratio, Threshold and operating voltages

I2- 0014

Complex magnetism and exchange interaction in $Nd_{0.8}Sr_{0.2}MnO_3$ manganite perovskite

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Abstract

Here, we report a detailed experimental study of the structural and physical properties of 20% Sr doped $NdMnO_3$, a complex oxide layered perovskite material a potential candidate for the applications in various fields. This particular composition has been chosen due to the recent observation of skyrmions in the $La_{1-x}Sr_xMnO_3$ system, setting an objective to explore new materials for the possibility of the stabilization of topological spin configurations. Through a combination of experimental techniques and rigorous theoretical analysis, the crystal structure, magnetic properties and exchange interaction of $Nd_{0.8}Sr_{0.2}MnO_3$ are systematically investigated. This work demonstrates the crucial role of structural parameters including lattice constants, Mn−O bond length, <Mn−O−Mn> bond angle, octahera rotation angle (θ), and complex interplay between structure and magnetic interaction in determining the magnetic properties in one of the layered perovskite materials, which we think is relevant to other materials that are comparable. Additionally, critical behavior of three-dimensional infinite-layer $Nd_{0.8}Sr_{0.2}MnO_3$ around the transition temperature (T_C) ≈ 145.54 K has been explored. We find that scaling exponents (β and γ) show non-trivial behavior which are in excellent agreement with the prediction of non-trivial systems having complex magnetic structures.

I2- 0015

Investigation of Structural, Transport & Magnetic Properties of Pyrochlore Iridates ($Gd_2Ir_2O_7$).

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Abstract

We have investigated the pyrochlore iridates' structural, electrical transport, and magnetic characteristics. Utilizing Rietveld analysis and x-ray powder diffraction, the structural examination was carried out. $Gd_2Ir_2O_7$ has a Fd3m space group and crystallizes in a cubic crystal form. $Gd_2Ir_2O_7$ is an anti-ferromagnetic, semi-metal-like insulator with a transition temperature of about 127K. Because Gd is in the +3 state and Ir is in the +4 state, this pyrochlore material has seven electrons in the 4f state and five electrons in the 5d state. Structural geometry is the source of dissatisfaction in pyrochlore structures. The primary magnetic attribute in this sample is the result of spin orbit coupling. This compound's insulator behavior is investigated utilizing the resistivity method with the four-probe method, and its antiferromagnetic nature is determined by magnetization versus magnetic field and inverse susceptibility vs temperature graph study.

I2- 0016

Crystal Structure analysis of 5,5'-(Furan-2-ylmethylene)bis(6-amino-1,3-dimethylpyrimidine-2,4(1H,3H)-dione)

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Abstract

The crystal structure of the title compound is determined by single crystal X-ray structure analysis. The compound $C_{17}H_20N_6O_5$, crystallizes in the monoclinic crystal system with space group $P2_1/c$ having unit-cell parameters: a=11.3123(8), b=14.8291(10), c=10.8777(8) Å, β=102.943(7), and Z = 4. The crystal structure was solved by direct methods using single-crystal X-ray diffraction data collected at room temperature and refined by full-matrix least-squares procedures to a final R-value of 0.0496 for 2109 observed reflections. The molecules in the crystal are linked into infinite two-dimensional network by C−H…O, C−H…N, N−H…O, N−H…N, and C−H…π type of hydrogen bonds. Molecules are also reinforced by π…π interaction between ring B and ring C, respectively.

I2- 0017

Study of Dispersion Characteristics of Spps At Metal/Lithium Niobate (Ferroelectric) Waveguide Structures

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Abstract

Surface Plasmon Polaritons (SPPs) are coherent electron-plasma oscillations at the interface of materials with opposite dielectric functions. No energy can be transferred from these oscillating charges to the far field in the dielectric. Energy cannot be freely transferred into the bulk of the metal either because of the electric field screening effect of the free electrons. Hence, this kind of waves can only propagate along the interface, with very high field confinement. This property has been used to fabricate extremely efficient plasmonic waveguides.

In this paper, we aim to investigate the behavior of surface plasmon polaritons at ($LiNbO_3$ /Ag/SiO_2) nano-waveguide structures. Since ferroelectric crystals have a permanent polarization, there is a distinct separation of charges on the two sides or two opposite domains of the $LiNbO_3$ crystal. This will result in an increase/decrease in electron density at the Ag-$LiNbO_3$ interface at the side with positive/negative charges, which will give rise to a blue-/red-shift of surface plasmon frequency. We observed a marked propagation length and geometrical/material dispersion properties here which ensure a sensitive plasmonic system operating at plasmon frequencies.

I2- 0018

Tailored $CuCoO_2$ nanostructure as supercapacitor electrode: Density functional theory and symmetric coin-cell

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Abstract

This work investigates the effect of alkaline condition on size of nanostructures and modification on the pseudocapacitive charge storage efficiency of $CuCoO_2$ nanostructures. Four samples were synthesized using a one-step facile hydrothermal technique at different alkaline conditions (NaOH, KOH, and LiOH), followed by structural, micro-structural, and chemical characterization using XRD, FESEM, BET, RAMAN, FTIR, UV-Vis and PL spectroscopy. Structural and microstructural studies illustrate monoclinic morphology of $CuCoO_2$ nanostructures with size in the range of ~300 – 500 nm, synthesized in the presence of higher NaOH concentration only, while a mixed phase of $CuCoO_2$ and CuO gets formed in other conditions. These samples exhibit specific capacitance in the range of **100-200 F g^{-1}** at scan rate 2 mVs^{-1} respectively with 6M KOH as electrolyte. High specific capacitance is attributed to the synergistic effect of higher surface area and faster charge transfer across $CuCoO_2$ electrode – KOH electrolyte interface. Most importantly, in spite of having low surface area in comparison with other nanostructures, the as-prepared nanostructures correspond to high specific capacitance. This phenomenon indicates the presence of highly active redox sites that facilitate charge transfer across the electrode – electrolyte interface. This investigation provides insights into the charge storage mechanism of $CuCoO_2$ electrode and its potential applications in energy storage devices.

J1- 0001

Investigating the Impact of Calcium carbonate and water on black soil Resistivity and geotechnical properties

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Abstract

This study examines the influence of calcium carbonate ($CaCO_3$) and water on the resistivity of soil and its subsequent effects on friction angle, plasticity, and cohesion. Laboratory experiments were carried out with varying $CaCO_3$ contents and moisture content. A factorial design varying
$CaCO_3$ concentrations (0-10%) and water content (0-50%) revealed significant correlations. Resistivity was measured with two-probe resistivity meter. Friction angle, plasticity and friction angle were measured using formulae depends on resistivity given in previous literatures. Results shows that increasing $CaCO_3$ content and water addition decreases soil resistivity, leading to reductions in friction angle and cohesion, while plasticity increases. These finding have significant implications for agricultural soil management, soil erosion control, and soil structure interaction.

J1- 0001

Impact of Gadolinium Phosphate ($GdPO_4$) and Various Cations (Li^+, Ca^{2+}, La^{3+}) on the NIR Reflectance of Bismuth Vanadate Pigment

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Abstract

This study explores the effects of $GdPO_4$ and a combination of Li, La, Ca, and Mo ions on the reflectance properties of Bismuth vanadate (BiVO4), a well-known yellow pigment, using scheelite-type solid solutions. The powdered pigments have a monoclinic scheelite (s-m) type structure. [(Li0.33Ca0.33La0.33)*x*Bi1-*x*][Mo*x*V1-*x*]O4 and (BiV)1-*x*(GdP)*x*O4. When $GdPO_4$ and the multi-ion system are incorporated into the $BiVO_4$ structure, a structural transition is brought about that impact the optical properties, such as bandgap tuning and absorption edge shifts. With particular colour coordinates displaying the most vivid hue at b* = 65.42 in the $GdPO_4$ system and b* = 78.32 in the multi-ion system, these pigments produce a range of intense yellow shades. They also have a high near-infrared reflectance, which makes them perfect for use as environmentally friendly and sustainable cool colourants in surface coating, paint, and plastic applications. These findings highlight the potential of [(Li0.33Ca0.33La0.33)*x*Bi1-*x*][Mo*x*V1-*x*]O4 and (BiV)1-*x*(GdP)*x*O4 as eco-friendly colorants for various applications which includes, surface coatings, paints.

J1- 0002

Synthesis of Copper Oxide Nanoparticles Using Leaf Extract of Cleistanthes Collinus its characterization and antibacterial study

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Abstract

The aim article to synthesis of copper oxide nanoparticles (CuO NPs) using leaf drug Clerodendrum infortunatum L.(Family : Lamiaceae) extract as a fuel by Co - precipitation method and their characterization. Xray diffraction studies showed that the particles are monoclinic in nature. The UV–visible absorption spectrum of CuO nano particle indicates the blue shift with increase of concentration of plant extract. The FTIR studies stretching vibration of the Cu-O bond in monoclinic CuO which is in close agreement with the previously reported work. The antibacterial activity shows unique mark.

The current study demonstrates convenient utilization of Clerodendrum infortunatum extract as a fuel for the efficient synthesis of CuO nanoparticles through a green synthesis method to obtain significantly physical and antibacterial activity.

Key Word: Copper Oxide, Nano particles, Leaf Extract, Characterization, Antibacterial Activity

J1- 0003

Synthesis and Electrochemical Performance of Fe based Composite material for Electrochemical Water Desalination Application

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Abstract

The primary need for each living being on the earth is potable water, and is tremendously growing with increasing population. To manage the higher demand for potable water, there are well established water desalination techniques such as distillation and reverse osmosis. All these techniques are highly energy intensive. The electrochemical water desalination technique is an emerging technique for water desalination requiring minimal energy input. Further, the development of efficient electrode material for electrochemical water desalination is crucial. Among several electrode materials, metal oxides showed higher specific capacitance and salt removal efficiency as compared to other electrode materials, In this study, we report the synthesis of Fe_3O_4/graphene composite and evaluate its electrochemical performance for electrochemical water desalination application. The composite material was synthesized through a hydrothermal method and characterized using galvanostatic charge-discharge technique to evaluate the electrochemical performance. The electrochemical characterization is performed in 1M sodium chloride aqueous solution as an electrolyte with three-electrode system at various current density values. At current density of 2 A/g, the specific capacitance of the Fe_3O_4/graphene composite display 230.2 F/g, indicating its potential as a high-performance electrode material for electrochemical water desalination application. The synergistic effects between Fe_3O_4 nanoparticles and the conductive graphene matrix contribute to the enhanced charge storage capabilities, demonstrating a promising electrode material for electrochemical water desalination system.

J1- 0004

Fabrication of All Liquid warm WLEDs with tunable properties for Artificial Lighting and Cancer Cell Imaging

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Abstract

WLEDs are now considered the cleanest and the cheapest energy sources and are increasingly in use for affordable illuminations of buildings and architecture. In recent times WLEDs have found extensive applications in indoor lighting, flat panel displays, bioimaging, and sensors and are successfully applied even as the headlights of automobiles instead of conventional sources which are known for hefty consumptions of gasoline and diesel. We have designed an environmentally friendly and innovative fluorescent system, proficiently capable of producing high-quality white light with CIE coordinates of (0.33, 0.35), a Colour Rendering Index (CRI) value of 84, and a Correlated Colour Temperature (CCT) of 5618K. The stoichiometric ratio of CQD, Fluorescein dye(linker), and Au Nanoclusters have been altered to generate white light emission. We believe that the most plausible mechanism behind such WL generation is cascaded energy transfer among the components. The incorporation of fluorescein dye has enhanced the energy transfer efficiency between C-dots to Au Nanocluster from 67% to 82 %. The retainment of optical properties was also obtained using the well-known agarose gel matrix. We believe that our proposed protocol for WLED fabrication holds promise for the development of diverse luminescent systems and also be applicable in the creation of turn-off and turn-on sensors for heavy metal ions.

J2- 0002

Effect of dielectric coating on the field emission performance of CNT – Si3N4 hybrids

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Abstract

The field emission phenomenon is an emerging process to achieve energy-efficient devices. Several materials like W [1], LaB6 [2], CNTs [3], etc., are being explored as field emission sources. CNTs have high electrical conductivity, high thermal conductivity, high tensile strength, large aspect ratio and other properties useful for emission applications. In the present study, pristine CNTs have been grown on a Si substrate using the Thermal CVD method followed by the Si3N4 coating with varying deposition time using PECVD method. Different characterizations were performed on all the samples to study the morphology, microstructure, elemental composition and electronic structure. Subsequently, field emission measurements were performed on all the samples and the highest current density of 8.2 mA/cm2 (30s deposited Si3N4 - CNTs) was achieved as compared to the 2.8 mA/cm2 (pristine CNTs). A thorough study of the field emission response of the samples disclosed that the enhancement in the current density had been obtained due to the decrement in the work function, increment in field enhancement factor, increased sp3 hybridised C atoms bonding, and the lowered screening effect. The study emphasizes the importance of the controlled deposition of dielectric over the CNTs and its effect on the field emission response.

Keywords: Carbon nanotubes, Field emission, CNT – Dielectric hybrids, Screening effect, Electronic structure.

J2- 0003

Photonic nanojet-assisted graphene-enhanced Raman spectroscopy

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Abstract

Recently, the photonic nanojet (PNJ)-assisted Raman microscopic technique has been found efficient in enhancing the Raman scattering signals of dye molecules and two-dimensional materials by tightly focusing the light beyond the classical diffraction limit of light. In this technique, the enhancement depends upon the radius and refractive index of the microsphere, the angle of incidence, wavelength light, the separation between the microsphere, and the complex refractive index of the substrate. On the other hand, the Graphene-enhanced Raman scattering (GERS) technique is found useful to enhance the Raman scattering signals of dye and protein molecules through chemical mechanisms instead of electromagnetic mechanisms. The GERS technique depends mainly on graphene-molecule separation, energy bandgap variation, electronic structure, and adsorption properties of probe molecules.
However, in both techniques, the signal-to-noise ratio is observed to be low for samples with ultralow concentrations. Therefore, there is a demand for a new technique to enhance the Raman signals of samples with ultralow concentrations. So, herein, we propose an efficient method named the PNJ-mediated GERS technique. This new technique can enhance the GERS signals by at least two orders of magnitude. More experimental details related to the PNJ-mediated GERS technique and the relevant experimental and theoretical results will be presented at the conference.

J2- 0004

Fabrications of Graphene Oxide and reduced graphene oxide Langmuir Blodgett Films an efficient SERS active Substrate

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Abstract

Surface Enhanced Raman Scattering (SERS) has become so powerful surface-sensitive technique because of its ability to detect minute amount of analyte molecules adsorbed on metal nanostructure. To fulfill these conditions, Langmuir Blodgett (LB) films play a vital role and have the unique flexibility to be used not only in lifting analyte monolayer molecules but also as robust and reproducible scaffolds in SERS spectroscopy. The Present work focuses on the LB films of Graphene Oxide (GO) and reduced Graphene Oxide (RGO) with impregnated silver nano particles (AgNPs) as noble SERS active substrates to detect the probe molecules at ultra low concentration**.** The as fabricated LB films were incubated in AgNPs for 24 hours to record the SERS spectra of analyte molecules. The self- assembly of GO and rGO has been conformed from FESEM and AFM data. The efficacy of the substrates as a SERS sensing platform was investigated for ultrasensitive detection of dye molecules like Rhodamine-6G (R6G) and 1,10 Phenanthrouline. The detection limit for R6G was upto 10^{-12} M and for 1,10 Phenanthrouline was upto 10^{-10} M. The present work may illuminate a pathway towards the fabrication of SERS-active substrates for the detection of dye molecules at lower concentrations and we believe that the as-prepared substrates can be further used to detect pesticides and in real-world diagnostic applications.

K1- 0001

Effects on the Solubility Limit, Structural, Magnetic and Electrical Properties of Rare Earth (Sm and Er) Co-substituted Cobalt Ferrites Nanocrystals

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Abstract

Rare earth (Sm and Er) co-substituted cobalt ferrites $CoFe_{2-2x}Sm_xEr_xO_4$ ($0 \leq x \leq 0.10$) were synthesized via the sol-gel method. The XRD patterns, FTIR and Raman confirmed the formation of a spinel structure. Secondary orthoferrites ($REFeO_3$) phases are formed from $x \geq 0.06$ samples. The Williamson-Hall method determined the crystallite sizes (D) and microstrain (ε). Rietveld refinement reveals a change in lattice constant (a), unit cell volume (V) and cation distributions with Sm-Er co-substitution. The initial magnetization (M-H) curves were analyzed using the law of approach to saturation (LAS) to determine the variation of the magnetic parameter, magnetocrystalline anisotropy (K_1), and saturation magnetization (M_s) in SmErCOF samples. An investigation of electron spin resonance (ESR) spectra reveals the interplay of the magnetic interaction and deviations of the Lande g-factors. A considerable increase in the dielectric constant values (ε') occurs from $x \geq 0.06$ samples. The ac conductivity displayed two distinct regions (I and II), consistent with Jonscher's double power law (JDPL). The temperature dependence frequency exponents (s_1 and s_2) suggest two conduction mechanisms: correlated barrier hopping (CBT) and non-overlapping small polaron tunneling (NSPT). The activation energies (E_a) obtained from multiple impedance representations were consistent with the electron hopping in Fe^{2+}/ Fe^{3+}. The Nyquist analysis indicates the dominance of the grain boundary resistance (R_{gb}).

K1- 0002

Enhancing Spin Polarization by Modifying Electron and Atomic Structure of Materials: A Theoretical Perspective

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Abstract

Enhancing spin polarization is crucial for the realization of spintronic devices that utilize the electron's spin degree of freedom in addition to its charge. This paper reviews theoretical methods for improving spin polarization based on modifications in the electronic and atomic structures of materials. Main approaches include doping, alloying, strain engineering, and interface manipulation, each of which may substantially alter the electronic band structure to improve spin polarization. Theoretical approaches, in particular DFT, provide valuable insight into these modifications on spin polarization. For instance, doping creates localized magnetic moments which interact with conduction electrons to favor the alignment of spins. On the other hand, strain engineering and interface manipulation modify the band structure and alter the spin-orbit interaction, enhancing further the polarization of spins.

Apart from electronic modifications, changes in atomic structure, such as the reduction in dimensionality of 2D material and the use of defect engineering, offer routes to achieve higher spin polarization. 2D materials, such as transition metal dichalcogenides, show quantum confinement phenomena and significant surface states involved with spin polarization. Defect engineering generates localized magnetic centers within non-magnetic hosts, leading to enhanced spin polarization.

New material systems, like topological insulators and 2D magnetic materials, now promise a new avenue for increasing the spin polarization. Theoretically, there are predictions that such materials, if doped or otherwise manipulated on the atomic level, can achieve near-perfect spin polarization. This review underlines the importance of theoretical approaches in guiding experimental activity in view of materials with optimized spintronic properties.

K1- 0003

Stearic acid infused Nano-Engineered Cu-Al composite Corrosion Resistant Superhydrophobic Coating on Steel Substrate by Electrodeposition

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Abstract

This study presents a comprehensive investigation into the development and characterization of nanotextured Cu-Al composite superhydrophobic coatings on steel substrate, modified with Stearic acid (SA). The aim was to enhance both hydrophobicity and anti-corrosion performance. By optimizing electrodeposition parameters such as voltage (25 to 30 V) and deposition time (5 to 15 min), we achieved a dense, uniform nano-structured rough coating of Cu-Al composite(SEM, Roughness analysis). This process significantly improved the water contact angle (WCA) from 32° to a remarkable 128°. Further modification with SA escalated the WCA to 152°(FTIR) while reducing the fractional surface coverage to 3.1%, illustrating a highly effective superhydrophobic surface. The coatings' anti-corrosion properties were investigated using Electrochemical Impedance Spectroscopy (EIS) and potentiodynamic measurements. Our findings demonstrate peak corrosion resistance at a 2 M concentration of Stearic Acid, achieving an impressive 98% anti-corrosion efficiency and low corrosion rate of mm/year, characterized by high polarization resistance and an enhanced charge transfer resistance of 95000 Ω-cm². The coating's robustness is attributed to its micro/nano-structured surface, which traps air and reduces water contact area and increase corrosion resistant behaviour

K1- 0004

Field induced assembly of microparticles for applications in micro-robotics

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Abstract

Micro-robotics using colloidal particles has advanced considerably due to its applications in targeted drug delivery, diagnostics, environmental remediation and industrial manufacturing1. Anisotropic colloidal particles, versatile in shape and material properties, are ideal candidates for functional micro-robots. By tuning the material properties and shape of the colloidal particles, they can be designed to respond to electric and magnetic fields, optical excitation and ion gradients in a controlled and desirable manner. Hematite (Fe2O3) being a canted antiferromagnet shows potential in targeted drug delivery since magnetic fields can penetrate the human body. With this purpose, we synthesized anisotropic hematite particles by a sol-gel method to attain super-ball (pseudo-cubic) and peanut shaped particles2. When exposed to an ac electric field, the peanut shaped particles can be made to re-orient along their long axis and stand upright. Subsequently when subjected to a rotating magnetic field, these particles can rotate in a plane perpendicular to the substrate, thus making a rotor in the micrometer scale. Cubic particles can be designed to form chain-like, or 2D structures by the application of magnetic and electric fields. Moving towards complexity- hematite cubes conjugated with TPM (3-methacryloxypropyl trimethoxysilane) spheres were synthesized to mimic a micro-engine with cargo. These micro-engines are propelled by photocatalytic breakdown of hydrogen peroxide under light and can be steered using magnetic fields. These anisotropic particles are ideal for developing active colloidal micro-rotors and complex structures with controlled reconfigurability, making them highly suited for next-generation micro-robotics in low Reynolds number environments.

K1- 0005

"Paper and Inks": Sustainable sensing through development of paper platforms

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Abstract

The platform of biosensor plays a pivotal role in the efficacy of detection, therefore the selection of an optimal material that meets all requisite criteria is essential. Paper as a platform for sensing application exhibit additive attributes over the other commercially available substrates as it fulfills the 'REASSURED' benchmark introduced under WHO guidelines. The study entails the fabrication of an electrochemical biosensing platform using regular office paper with different GSM thickness (75, 85,120 and 140 GSM). The conductive inks, paper thickness, design pattern, hydrophobic layer and connection materials were iterated and optimized through multiple scans of cyclic voltammetry. A simplified design with reference and working electrode with an optimized distance of around 3mm, resulted in reduced ohmic resistance. The concentration and number of layers of conductive inks were optimized through conductivity measurements which lie between 1Ω to 4 Ω for reference electrode, 0.0005 MΩ to 0.025 MΩ for counter electrode and 0.1 kΩ to 1.2 kΩ for working electrodes. Beside this an ecofriendly volatile organic compound free hydrophobic reagents were utilized for fabricating the sensing region. The CV scans shows stability of adsorbed materials on the fabricated paper platform stating that the platform could be further evaluated for biosensing application.

K1- 0006

Effect of Li^+ - ion and nano crystallite size on zeta potential and electrical studies in SBNN ferroelectric materials for device applications

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Abstract

Non - toxic polycrystalline TB – type ferroelectric ceramic materials are found to be technologically important materials for device applications due to their high dielectric constant, piezoelectric and electro-optic properties. The present investigation is Li^+-ion modified and unmodified TB- type ferroelectric ceramic materials are specifically Li^+ - SBNN (x = 0.0 to 1.0) prepared by conventional solid state reaction high temperature sintering method and using high purity oxides and carbonates. The influence of monovalent alkali lithium ion and nano-crystallite size on zeta potential, micro structural, dc electrical resistivity and piezoelectric properties are studied in Li^+: SBNN ceramics and reported. The present ceramic system is single phase orthorhombic (mm2) structure reported by XRD and the average nano crystallite size has been measured by Scheerer's formula. The dc electrical resistivity is a function of temperature and reported that PTCR nature suitable for pyroelectric and piezoelectric device applications.

K1- 0007

Up-conversion luminescence of Zn^{2+} co-doped Y_2O_3: Er^{3+}/ Yb^{3+} nanophosphor for temperature sensing application

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Abstract

The Zn^{2+} ion enhanced up-conversion emission of Y_2O_3:Er^{3+}/Yb^{3+} nanophosphor was synthesized through hydrothermal method. The crystal structure, phase purity and morphology of the phosphor were characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and Transmission electron microscope (TEM). The incorporation of Zn^{2+} ions into Y_2O_3:Er^{3+}/Yb^{3+} has shown significant enhancement in the green (525 nm and 550 nm) and red (665 nm) emission bands under 980 nm laser excitation. The materials were further investigated to understand the dependence of excitation power density on temperature sensing and optical heating behavior using the fluorescence intensity ratio technique from the two thermally coupled energy levels ($^2H_{11/2}$ and $^4S_{3/2}$) of Er^{3+} ions. The obtained result indicates that the present material is suitable for optical thermometry as well as for making infrared to visible up-converting devices.

K1- 0008

New Trends in Skin Friendly and Comfortable Electronics

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Abstract

Day by day as electronic devices are being miniaturized, made more light weight, wearable, and intelligent, we are entering into an era where electronics in ultra-thin, soft, flexible and stretchable form has no longer been a dream and is becoming a reality. A new branch of electronics known as skin friendly electronics has thus emerged in recent years and gaining attention of the researchers across the globe. As demand for human-machine interfaces is surging, developing materials having high-performance sensing capabilities is seeing a steep rise and to meet out this, researchers are making efforts to fabricate flexible, stretchable, comfortable and wearable materials which responds to various stimuli such as strain, stress, pressure, temperature, humidity etc. and generate signals due to change in resistance, voltage, current, or capacitance etc. In the present review, we incorporate the recent trends and progress in skin friendly materials their fabrication aspects and prospective applications. Skin friendly electronic materials comprising of piezoresistive, piezoelectric, thermoelectric, conductive polymer, carbon nanomaterials etc. are analyzed here. In the end, practical applications of skin friendly electronic materials in fields of human healthcare, human motion detection, tactile perception and human-machine interface are discussed.

Key words: human-machine interface, piezoresistive, piezoelectric, thermoelectric, Skin friendly electronics, strain

K2- 0001

Future Applications of Junctionless Transistors Using Gallium Phosphide Channel for the Semiconductor Industry

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Abstract

Gallium phosphide (GaP) is a semiconductor substance with several uses in optical systems. For the preparation of GaP, a number of solution-based key reactions have been established over the past 20 years. These techniques include various solution-based pathways and the thermolytic and metathetical processes. Additionally, applications for III–V GaP based quantum dots in bioimaging and gas sensing are established. Indirect band gap semiconductors, or GaPs, are utilized in microelectronic applications. A two-GaP nanowire optical X-coupler that enables signal spectrum separation can be created. The work's findings provide new avenues for using GaP nanowires in sophisticated photonic logic circuits and nanoscale interferometers. This work presents a thorough examination of the electrical characteristics of a junctionless gate-all-around field effect transistor design with a silicon channel and gallium phosphide (GaP) as the III-V compound material. The simulations showed that when compared to other circuit topologies, GaP had a more favorable subthreshold slope and reduced drain-induced barrier lowering (DIBL). Additionally, a strong association was found in the study between the values of drain-induced barrier lowering (DIBL) and subthreshold slope (SS) in gallium phosphide (GaP). At 67.84 mV/V, the subthreshold slope is quite close to the optimum value of 60 mV/V and the drain-induced barrier lowering (DIBL) of roughly 22.50 mV/dec.

K2- 0002

Electrical properties of Au/n-GaN Schottky diode (SD) modified using a high-k dysprosium oxide (Dy_2O_3) insulating layer

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Abstract

This work focuses on employing the e-beam evaporation method to fabricate a metal/insulator/semiconductor (MIS) diode, specifically an Au/Dy_2O_3/n-GaN diode with a high-k rare earth oxide (Dy_2O_3) interlayer. The MIS diode's current-voltage (I-V) characteristics were analyzed to evaluate its electrical properties, and the results were compared to those of the Au/n-GaN Schottky diode (SD). The current-voltage (I-V) characteristics of the MIS diode demonstrate that it possesses superior rectification properties and lower reverse leakage current as compared to the SD. From the I-V characteristics, the barrier height (Φ_b) and ideality factor (n) for the SD and MIS diode are 0.82 eV and 1.43 and 0.91 eV and 1.17, respectively. The insertion of a Dy_2O_3 layer between the Au electrode and the n-GaN substrate increases Φ_b while decreasing leakage current. The electrical parameters Φ_b, n, and RS are also evaluated using the methods developed by Cheung and Norde. The Φ_b values derived from the I-V, Cheung's, and Norde's approaches are almost similar, indicating their validity and effectiveness. The reduction in the calculated interface state density (N_{SS}) of the MIS diode may be attributed to the efficient passivation of the GaN surface by the Dy_2O_3 layer, resulting in a decrease in N_{SS}. The Poole-Frenkel emission is the leading current transport at a lower bias, though Schottky emission (SE) is governed by the current transport at a higher bias of the SD. However, the SE is dominant by the current transport in the MIS structure.

K2- 0003

Effect of ionized impurities on low field electron mobility in GaN

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Abstract

Gallium Nitride (GaN) is an important wideband gap semiconductor with applications in high frequency, high-temperature, and high-power microelectronic devices. Scattering of charge carriers from various sources present in the material affects the material's transport properties. So, it is imperative to account for sources of scattering present in GaN and to comprehend their impact on the drift electron mobility.
In this paper, we report the drift electron mobility of GaN, estimated analytically considering the likely sources that are relevant for GaN grown hetero-epitaxially on foreign substrates like sapphire or SiC. The effects of ionized impurities, neutral impurities, dislocation defects, acoustic phonons (deformation potential and piezoelectric potential), and optical phonons on the electron mobility in GaN have been estimated as a function of temperature. A comparison of the models proposed by Conwell -Weisskopf (CW) and Brooks- Herring (BH) for ionized impurities revealed that both of the models are in good agreement for temperatures below 50K. The variation in estimated mobility at temperatures above 50 K is attributed to the quantum mechanical nature of BH model. It was observed that the dominant scattering mechanism affecting the drift electron mobility of GaN are scattering due to optical phonons and ionized impurities at temperatures above 50 K. The resultant electron mobility at 300K for impurity ~10^{16} m^{-3} is estimated to be ~ 100 cm^2/Vs. Higher impurities levels degrades the mobility further. The estimated results for room temperature are in good agreement with experimentally measured mobility in GaN.

ey word: GaN, Ionized impurity, scattering rate, Mobility.

K2- 0004

Electrical Modulation of Metal-Semiconductor States in 2H-MoTe2

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Abstract

In this work, we demonstrate tunable semiconducting and metallic behavior in 2H-$MoTe_2$ through electrical control of Joule heating, unlike other studies focusing on structural phase transitions for such changes. At low voltages, the material exhibits semiconductor behavior, but at higher currents, it changes to a metallic-like state, as shown by an increase in resistance with temperature. Voltage and temperature-dependent Raman studies confirm that this transition occurs without structural changes. We validate our hypothesis that the metallic behavior is driven by phonon scattering through experiments involving hydrogen gas and laser exposure. In the metallic state, hydrogen exposure increases resistance due to phonon scattering, while laser exposure shows no significant effect. These phenomena are reduced when 2H-$MoTe_2$ is combined with a hexagonal boron nitride/multilayer graphene substrate, which acts as a heat sink. This dynamic control of conductivity underscores the potential of 2H-$MoTe_2$ for advanced nanoelectronic applications.

K2- 0005

Raman study of Ni negative ions implanted Indium Phosphide

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Abstract

Indium Phosphide is a direct band gap semiconductor. This semiconductor has found potential application for optoelectronics devices like laser diodes and photonic integrated circuits for the optical telecommunications industry. Ion implantation is a process by which energetic ions can be introduced into a single crystal substrate in order to change its surface, optical, structural, and electrical properties. The depth to which the energetic ions (dopants) are implanted primarily depends on the energy of the ion beam. The Ni negative ion implantation in semiconductor forms diluted magnetic semiconductors (DMS). The negative ion implantation technique remarkably improves the charging problem since the incoming negative charge of implanted negative ions is easily balanced by the outgoing negative charge of a part of secondary electrons [1].

In the present work 100 keV Ni negative ions were implanted into InP for different ion fluences ranging between 5 x 10^{15} and 1 x 10^{17} cm^{-2} at room temperature using SNICS ion source at Low Energy Ion Beam Facility (LEIBF) at Inter University Accelerator Centre (IUAC), New Delhi. Ion beam scanning was used to implant the whole sample surface in a uniform way. The optical properties of non-implanted and samples implanted with Ni negative ions were investigated by using the Raman spectroscopy. The Raman spectra of non-implanted Indium Phosphide showed two peaks at 301.62 cm^{-1} and 342.48 cm^{-1}, which was assigned to TO and LO Raman modes respectively. The TO and LO Raman modes were also observed in Ni negative ion implanted Indium Phosphide samples. For ion fluences 5 x 10^{15} and 1 x 10^{16} cm^{-1} the TO and LO modes were observed at 298.97 cm^{-1} and 338.53 cm^{-1} respectively, however for ion fluence 5 x 10^{16} cm^{-1} the TO and LO mode were observed at 300.29 cm^{-1} and 339.85 cm^{-1} respectively. Further for ion fluence 1 x 10^{17} cm^{-1} the TO and LO modes were observed at 297.65 cm^{-1} and 335.90 cm^{-1} respectively. This shifting of peak positions with ion fluence indicates the presence of stress in the implanted samples. The intensity of the Raman peaks was found to change with ion fluence. This indicates the presence of defects in the implanted samples.

K2- 0006

Synthesis and Characterization of Cu:Ni Co-doped ZnO Thin Films for its Optoelectronics Applications

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Abstract

Since last two decades ZnO-based thin films and nanocomposites have found ever growing interest as novel material with their unique electrical, optical, catalytic, piezoelectric, electrochemical and biomedical properties. The multifunctionality and tunability makes it a most promising material to scientific community for its device applications. The efficient use of ZnO based advanced devices, intensively requires the appropriate strategy for synthesis and characterization of this material of different dimension such as thin films, nanoparticles, and amalgamation of other organic and inorganic materials using sophisticated techniques. The present paper reports the synthesis and characterization of Cu:Ni co-doped ZnO thin films for its optoelectronics applications using sol-gel spin coating system. The synthesized thin films were characterized for its structural, optical and chemical characteristics using XRD, UV-Vis, and FTIR spectrometer. Thin films of ZnO were successfully synthesized with different co-doping of Cu/Ni using sol-gel spin coating technique. The XRD patterns revealed that all the films have crystalline nature with a hexagonal structure. The optical absorption spectra were measured using UV-Vis spectrometer. The energy band gap (E_g) of pristine ZnO thin films found to be 3.23 eV, and it decreases with increasing the Cu:Ni concentration in to ZnO matrix. Measurements revealed that the film absorption coefficient, optical band gap and Urbach energy varies with the Cu:Ni doping concentration. The Fourier transform infrared spectroscopy (FTIR) of ZnO films confirms the presence of various functional groups in the deposited thin films.

Keywords: ZnO thin films, Optical materials, Semiconductor Materials, Sol-gel Spin Coating System, Optoelectronic Devices

L1- 0001

Dielectric Dispersion Analysis of Quaternary Ceramic BNT-BT-PMN-PT

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Abstract

A quaternary solid state solution with MPB composition, [$0.47(Bi_{0.5}Na_{0.5})TiO_3$-$0.04BaTiO_3$-$0.31Pb(Mg_{1/3}Nb_{2/3})O_3$$0.18PbTiO_3$] has been synthesized using solid state reaction method by incorporating BNT-BT relaxor into the PMN-PT ferroelectric material to explore the combined advantages of relaxor and high Curie temperature ferroelectric materials. This combination also eliminates the pyrochlore phase and reduces the lead content.

Dielectric dispersion analysis on this quaternary ceramic was carried out in the frequency range of 200 Hz to 2 MHz with different temperatures ranging from 30 ^oC to 300 ^oC. The low frequency dielectric constant was found to increase with temperature, which reaches to its maximum value of about 5000 at 170 ^oC and then decreases with further increase in temperature. Debye type relaxation was clearly observed in its both ferroelectric and paraelectric phases. Two Debye peaks in dielectric loss vs frequency curves were observed in the temperature range 125 ^oC to 175 ^oC. These peaks show a shift towards higher frequencies with increasing temperature. The dielectric dispersion in both the ferroelectric and paraelectric phases could be explained using Debye distribution of relaxation times but the distribution parameters were significantly different in two phases. This difference has been attributed to the changed interaction among species in two phases.

The high dielectric constant, low dielectric loss, less variations in dielectric parameters with temperature and absence of DC conductivity make this material a good candidate for a wide variety of applications, including multilayer capacitors, actuators, sensors and transducers etc.

L1- 0002

Dielectric dispersion and electrical properties of YNaSiO compounds doped with Tb ions

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Abstract

In this paper, auto combustion method was employed to synthesize the $Y_{9-x}Na(SiO_4)_6O_2$: xTb, where x = 0, 0.1, 0.2, 0.3 (YNaSiO: xTb) oxy-apatite compounds. The Hexagonal phase with space group p63/m was confirmed by x-ray diffraction analysis of the synthesized compounds. The microstructure of the YNaSiO: xTb compound was obtained by scanning electron microscopy. The crystals are random in shape and irregular in distribution. The presence of chemical bonds between the elements of the compounds and functional groups are confirmed from the transmission spectra obtained through Fourier Transform Infrared (FTIR) Spectroscopy. The frequency (10^2 Hz – 10^2 kHz) dependent dielectric studies of the YNaSiO: xTb compounds were done for different temperatures. The dielectric constant and dielectric loss decreased with increasing values of external field's frequencies due to reduction of polarization effects. The alternating conductivity analysis showed dispersion with increasing values of frequency, and followed universal jonscher's power law. These results suggest the utilization of YNaSiO: xTb compounds in electrical devices as loss component, capacitors etc.

L1- 0003

Investigation of structural, dielectric and electrical properties of $MgCr_{2-x}O_4$: xFe (x = 0.6, 0.8) chromites

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Abstract

In this paper, the properties of $MgCr_{2-x}O_4$: xFe (x = 0.6, 0.8) chromite synthesized via solution combustion route were investigated. The X-ray diffraction (XRD) analysis confirmed the crystal structure and phase formation of the materials. The FTIR spectroscopy was used to obtain the transmittance spectra which determined the bands around 563 cm^{-1} and 668 cm^{-1}, corresponding to the stretching and bending vibration of metal oxide bonds. The dielectric properties including dielectric constant (ε'), dielectric loss (ε'') and ac conductivity were examined using the dielectric spectroscopy over a frequency range of 100 Hz – 100 kHz at different temperatures. The value of dielectric constant decreased with frequency owing to the ceasing effect of polarization. The dielectric parameters (dielectric constant and tangent loss) have been interpreted according to Maxwell-Wagner's model on the basis of space charge polarization. The behaviour of AC conductivity increased with an increase in frequency and temperature due to hopping of charge carriers between Cr^{2+} and Cr^{3+} ions. The single semicircle arc observed in the cole – cole plot suggested that the non – Debye relaxation present in the sample. The obtained result shows the capability of materials for developing the electronic devices, electrode materials, ceramic capacitors and energy storage devices, etc.

L1- 0004

Investigation of Dielectric Properties of $Ca_{6-x}Na_2Y_2(SiO_4)_6(Cl)_2:xGd^{3+}$ Compounds

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Abstract

The dielectric properties of $Ca_{6-x}Na_2Y_2(SiO_4)_6(Cl)_2:xGd^{3+}$ (x = 0 – 0.05 mol%) chlorapatite compounds synthesized by hydrothermal method has been reported here. The formation of monoclinic phase with space group $P2_1/c$ has been confirmed by P-XRD. The investigation of dielectric parameters depending on frequency and temperature reveals that the space charge polarization plays dominant role whereas, the contribution of grains and grain boundaries has been indicated through complex impedance spectroscopy. The NTCR behaviour has been observed in the compounds as the resistance of grain and grain boundary decreases with increase in temperature. The electrical transport due to long range and short range hopping of charge carriers in low and high frequency region respectively has been indicated by electrical modulus spectroscopy. The a.c. conductivity spectrum disperses with increase in frequency which shows that the compound obeys Universal Jonscher's power law and can be used in capacitors and biological field.

L1- 0005

Investigation of structural, dielectric and ferroelectric behaviour of MnO2 modified (Ba0.85Ca0.15)(Zr0.1Ti0.9)O3 ceramics

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Abstract

The purpose of this work is to study the structural, dielectric and ferroelectric properties of MnO2 doped (Ba0.85Ca0.15) (Zr0.1Ti0.9)O3 lead free ceramics at varying weight percent. X-ray diffraction was used to study the structural estimation and the results show that all compositions have dual phase crystal structures i.e tetragonal + orthorhombic with space group P4mm+ Amm2. Raman spectroscopy indicates the sifting of peak and modification in the FWHM of the corresponding spectra was noticed from the deconvolved peaks using the Lorentz function. The temperature-dependent dielectric data shows that dielectric permittivity falls as Mn concentration increases whereas no much variation was observed in the transition temperature. The dielectric loss was found to be diminish with increase in Mn concentration. The diffusivity parameters were found from the modified Curie-Weiss Law and the diffusivity increases with doping percentage. A well-saturated ferroelectric loop is obtained for all compositions with a reduction in the remnant polarization and coercive electric field with increase in Mn concentration.

L1- 0006

Dielectric and Raman Spectroscopic Properties of High Dielectric and Metamagnetic Eu_2CoMnO_6 Mixed Perovskite

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Abstract

Monophasic and polycrystalline mixed perovskite Eu_2CoMnO_6 is synthesized by fine tuning of solid state chemical synthesis route. Rietveld refinement of the X-ray diffraction analysis of the prepared compounds confirmed Eu_2CoMnO_6 adopted monoclinic $P2_1/n$ space group with estimated lattice parameters $a = 5.333$ Å$, b = 5.565$ Å$, c = 7.582$ Å$, \alpha = 90.0°, \beta = 89.99°$ and $\gamma = 90°$. Temperature and frequency dependent dielectric properties are investigated for a wide temperature $(80 - 350\ K)$ and frequency $(1\ kHz\ -\ 1\ MHZ)$ ranges. Reasonably high value of dielectric permittivity $(\sim 10^3)$ around ambient temperature, and particularly in the kHz frequency regime, associated with relatively weak temperature sensitivity is an attractive feature with application prospects in high dielectric devices. The observed broad and asymmetric dielectric relaxation peak in the electric modulus spectra deviates considerably from the ideal Debye type dielectric relaxation which can be ascribed to the influence of compositional inhomogeneity and anti-site disorder. The observed high permittivity is attributable to the hopping polarization contribution of two dissimilar cations 'Co' and 'Mn' in the 'B'-sites of the mixed perovskite Eu_2CoMnO_6. The influence of the anti-site disorder is evident in the Raman active modes detected around 498, 628, and 1250 cm^{-1}. Magnetic properties revealed, a magnetic transition in temperature variation in the DC magnetization observed around $T_c = 120\ K$. Interestingly, a correlation of magnetic transition to dielectric relaxation was also observed. Below T_c, the dielectric constants merges to a low value for all the measured frequencies. Frequency dispersion is only appreciable at the magnetically disordered paramagnetic phase.

L1- 0007

Dielectric Relaxation of $(Bi_{0.2}Na_{0.2}Ba_{0.2}Sr_{0.2}Ca_{0.2})TiO_3$ High-Entropy Ceramic

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Abstract

In materials design, entropy is a crucial parameter like enthalpy. However, it was not considered until the concept of High Entropy Materials was introduced. High entropy materials are a relatively young new class of materials that were discovered in 2003. It possesses four kinds of special core effects such as (i) High entropy effect, (ii) Severe lattice distortion effect, (iii) Sluggish diffusion effect, and (iv) Cocktail effect. The High entropy Ceramics (HECs) are the solid solutions of inorganic compounds (five or more cations or anions sublattices) with one or more Wykoff sites shared by equal or nearly equal atomic ratios of multi-principal elements. HECs have gained the attention of researchers due to their fascinating properties**.** In this report, the synthesis and functional properties of an A-site disordered high entropy perovskite $(Bi_{0.2}Na_{0.2}Ba_{0.2}Sr_{0.2}Ca_{0.2})TiO_3$ ceramic is presented. The Rietveld refinement of the XRD pattern and SEM-EDS confirmed the single-phase solid solution with a tetragonal crystal structure. A detailed study of the dielectric behavior of the sample was done. Curie-Weiss law and modified Curie-Weiss law were fitted to the relative permittivity. In addition to this, Vogel-Fulcher law was also fitted to confirm the relaxor behaviour of the studied material, and the freezing temperature (T_f) is found -18℃. HECs are highly tolerant to ions and their properties can be tailored by composition variation.

L1- 0008

Studies on Effect of Incorporation of Granite Waste (Gujarat, India) in Replacement of Feldspar on Fired Properties of Glazed Vitrified Tile Body Formulation

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Abstract

Indian Granite industry generates a lot of waste during its processing. In the present study, the effect of incorporation of granite mining waste in replacement of two types of feldspars, (one containing both potash and soda and the other containing only soda) being used in a glazed vitrified tile body formulation is undertaken to utilize maximum waste. Feldspar is an important raw material used in glazed vitrified tile body formulation in bulk quantity (50-60%). Granite samples and feldspar samples were characterized by wet chemical analysis and XRD. Ground granite sample was incorporated in replacement of two types of feldspar in vitrified tile body formulation in two steps and bar sample specimens were prepared by pressing. Samples were fired under industrial firing conditions (temperature-1203°C- Firing cycle-57 Minutes) and fired characteristics such as fired shrinkage, fired modulus of rupture, breaking strength, water absorption, and bulk density were studied. XRD of the fired samples was also carried out. Results showed that the replacement of feldspar containing both potash and soda resulted in only marginal change in fired shrinkage, water absorption and bulk density. However, the complete replacement of feldspar (both types) resulted in slight increase in fired shrinkage and water absorption as compared to the reference body without granite waste. Results revealed that after partial and complete replacement of feldspar by granite waste, all the fired properties of tile specimens confirms to BI a and BI b group respectively as per IS 15622:2017.

L1- 0011

Studies on structural, electrical and magnetic properties of divalent transition metalions substituted lithium ferrite synthesized by ceramic Technique.

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Abstract

Lithium Ferrite with compositional formula $Li0.5Fe_2O_4$ substituted with divalent transition metal ions such as Ni2+, Co2+, Zn2+ ions were synthesized via conventional ceramic technique using high energy ball milling technique. The synthesized ferrite underwent calcination at 650^0C for 1h and sintered at 950^0C for 2h. Na2SiO3 and V2O5 were added as sintering aids. Structural studies were done using X-ray diffraction (XRD) technique and confirmed the formation of a single-phase spinel structure in all prepared samples. From the XRD data, structural parameters including lattice constant, crystallite size and X-ray density were determined. FTIR examined additional structural information such as metal oxygen bonds present in the sample. Scanning electron microscopy (SEM) gives information on the microstructural information revealing grain size and grain distribution etc. The frequency dependence of the electrical properties such as dielectric constant, dielectric loss, real and imaginary impedance, nyquist plot were studied. Magnetic hysteresis properties of the samples were explored using a vibrating sample magnetometer (VSM). From the studies the various hysteresis parameter such as remanance, coervity for the different ferrites were The results of the studies have been presented in the paper.

Keywords: Lithium ferrites, XRD, SEM, dielectric properties, M-H loop

L1- 0012

Structural and photoluminescence properties of Er^{3+} doped $SrBi_2Ta_2O_9$ ceramics

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Abstract

This study examined the structural and photoluminescence properties of polycrystalline Er^{3+}doped $SrBi_{2-x}Ta_2Er_xO_9$ ceramics synthesized using the conventional solid-state reaction method. Variations in the doping concentration (x = 0.00, 0.02, 0.04, 0.06, 0.08) were explored to assess their impact on luminescence and structural characteristics. X-ray diffraction (XRD) analysis was used to confirm that the samples had a single-phase orthorhombic structure with space group A21am after heat treatment that included calcination at 900°C and sintering in the 1100–1150°C temperature range. Scanning electron microscopy (SEM) images revealed the formation of highly dense plate-like microstructures in the sintered pellets. Furthermore, the photoluminescence (PL) spectra were studied at specific excitation wavelengths of 488nm, highlighting the enhanced luminescent properties attributed to Er^{3+} doping. This research underscores the potential of rare-earth-doped ferroelectric ceramics in various energy-related applications, including optoelectronics and sensing technologies.

Keywords: Solid-state reaction method, Photoluminescence, X-ray diffraction, Scanning electron microscopy, Ferroelectric Ceramics

L1- 0013

Synthesis and Characterization of Magnesium Oxide (MgO) Nanoparticles via Wet Chemical Approach

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Abstract

Magnesium nitrate hexahydrate [Mg(NO3)2·6H2O] with 98% purity, sourced from Loba Chemie, and distilled water were utilized to synthesize magnesium oxide (MgO) via a wet chemical method. In this approach, magnesium nitrate served as the precursor, while distilled water acted as the solvent. The synthesized MgO samples were characterized using Thermogravimetric Analysis (TGA), X-ray Diffraction (XRD), UV-Visible (UV-Vis) spectroscopy, and Fourier Transform Infrared (FTIR) spectroscopy. The average crystallite size is determined through XRD using Scherrer's equation and it is found to be approximately 16 nm. The energy band gap is studied by using UV-Vis spectroscopy and it is calculated 5.03 eV for the synthesized MgO nanopowders. This study contributes to advancing experimental research on the physical properties and potential applications of MgO nanopowders, particularly in areas such as high-density ceramics, bactericidal additives, and refractory materials. The details results will be presented and discussed.

L1- 0014

Room Temperature Dielectric and Ferromagnetic behavior of Vacuum Annealed (1-x)Bi($Zn_{0.75}W_{0.25}$)O_3-x$PbTiO_3$ Ceramics

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Abstract

Polycrystalline solid solutions of (1-x)$PbTiO_3$-(x)Bi($Zn_{0.75}W_{0.25}$)O_3[x=0.10, 0.20,0.30] have been prepared by using solid state reaction method and followed by air annealing (AA)/ vacuum annealing (VA). All the prepared samples exhibit single phase perovskite structure with tetragonal symmetry (*P4mm*). Structural parameters are calculated using Rietveld refinement technique. The surface morphology of all the samples is recorded by using Scanning Electron Microscope (SEM) at room temperature. The influence of VA on dielectric parameters such as dielectric constant and tangent loss of the samples are studied and compared with that of AA samples. The results showed better dielectric properties of VA samples as compared to AA samples. Interestingly, the VA samples also exhibit unusual ferromagnetic property in non-magnetic $PbTiO_3$-Bi($Zn_{0.75}W_{0.25}$)O_3 samples, transforming these into room temperature magnetoelectric multiferroics.

Keywords: Vacuum annealing, Rietveld refinement, Dielectric constant, Multiferroics

L1- 0015

Effect of Holmium Doping On Structural and Luminescence Characteristics in $BaBi_2Nb_2O_9$ Ferroelectric Ceramics

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Abstract

A comparative study of pure and holmium doped $BaBi_2Nb_2O_9$ ceramics was carried out. The samples were synthesized by the solid state reaction method. In this study we investigated the structural and luminescence properties of pure and Ho-doped $BaBi_2Nb_2O_9$ ceramics. X-ray diffraction (XRD), photoluminescence and scanning electron microscope (SEM) analysis are employed to characterize the samples. The ceramics underwent heat treatments including calcination at 950°C followed by sintering at 1050°C. X-ray diffraction confirmed the formation of single-phase orthorhombic structure with no secondary phase. Scanning electron microscopy (SEM) reveals a randomly oriented plate like microstructure with non-homogeneous grains. Furthermore, PL spectra were examined at 455 nm excitation wavelengths to emphasize the improved luminous property caused by doping of Ho3+..The results indicate significant modifications in the material's properties, which can be tailored for specific applications.

Keywords: Ceramics; Ferroelectrics; Photoluminescence; solid state reaction method

L1-0016

Electron Density Distribution and Microstructural Study of Spark Plasma Sintered $BaZr_{0.85}Ho_{0.10}Y_{0.025}Nd_{0.025}O_{3-\delta}$ Electrolyte Ceramic for Intermediate Temperature SolidOxide Fuel Cell Applications

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Abstract

Highly dense $BaZr_{0.85}Ho_{0.10}Y_{0.025}Nd_{0.025}O_{3-\delta}$ electrolyte ceramic membrane for intermediate-temperature solid oxide fuel cells is synthesized using a cost-effective flash pyrolysis method followed by spark plasma sintering at 1500 ℃ for 20 min. The sintered pelletis characterized using various techniques like high resolution X-ray diffraction (HRXRD) andfield emission scanning electron microscopy (FESEM). The XRD pattern of sintered pellet shows the pure cubic phase with $Pm\bar{3}n$ space group symmetry through the Rietveld refinement. The examination of electron density distribution, calculated by the maximum entropy method (MEM), verifies the presence of oxygen vacancies at the octahedral site in theBZHYN. The microstructure of the fracture surface of the sintered sample indicates highly dense with a relative density of 98.8% through FESEM.

L2- 0001

Negative Local Partial Density of States

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Abstract

We determine local objects of density of states of hierarchy like partial density of states, local partial density of states, injectivity, emissivity, etc.,-which is provided by Larmor clock theory-in quantum systems like mesoscopic systems. These local objects are determined by the scattering phase shift, which is related to scattering matrix element. Theoretically, it has been shown earlier. In this work, we discuss some theoretical experiments that can be done to observe and confirm negative local partial density of states. We target only experimental expressions, which are given by the Landauer-Buttiker three-probe conductance setup. The Larmor clock theory can be studied by functional analysis as it involves functional derivative of scattering phase shift with respect to local potential at the local coordinate. This mathematical study reveals many new results like the negativity of local partial density of states, Fano resonances, the possibility of time travel, etc. We establish theoretical experiment with the study of Argand diagram, Burgers circuit, abrupt phase drops which falls under functional analysis. This study bypasses the axioms of quantum mechanics.

L2- 0002

Topological nodal line features in NiSe semimetal: Insights from electronic transport and DFT studies

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Abstract

The unique linear band touchings at one-dimensional lines or rings characteristic of the nodal line semimetal phase have generated significant research interest, particularly for potential applications in low-dissipation electronics and spintronics. In our study, we investigated these phenomena in a single crystal of NiSe by analyzing temperature-dependent resistivity data, which we fitted using the Bloch-Gruneisen-Mott formula to identify various scattering processes, including electron-phonon interactions and Mott's interband scattering. Our findings were corroborated by transverse magnetoresistance (MR) measurements, which followed extended Kohler's rule and showed deviations from Kohler's rule, further confirming the presence of multiple scattering mechanisms. The temperature-dependent resistivity under varying magnetic fields revealed NiSe's topological semimetallic properties. The observed negative magnetoconductivity, which was analyzed using the Hikami-Larkin-Nagaoka equation, indicated weak antilocalization. The weak field magnetoconductivity followed an $-ln(B)$ scaling behavior, consistent with the topological nodal line feature. Density functional theory (DFT) calculations suggested a slight predominance of electron concentration over hole concentration. Non-linear Hall resistivity data with a negative slope also pointed to electron dominance. It is plausible that the low magnetoresistance might be due to the slightly larger size of electron pockets compared to hole pockets. DFT calculations identified five types of nodal lines with a π-Berry phase, absent spin-orbit coupling (SOC): one infinite, one diamond-shaped, two with six-fold, one with three-fold rotational symmetry. All nodal lines are oriented perpendicular to the *c*-axis, except for the diamond-shaped one. The DFT results also showed that two of these nodal lines remain protected even when SOC is present.

L2- 0003

Synthesis and structural characterization of $Bi_{1.21}Tb_{0.04}Sb_{0.75}Te_{1.3}Se_{1.7}$ magnetic topological insulator single crystal

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Abstract

Topological insulators (TIs) are novel materials characterized by an insulating bulk and time-reversal symmetry (TRS) protected conductive surface states. 3D TIs, like Sb_2Te_3, Bi_2Te_3, and Bi_2Se_3, are narrow-gap semiconductors with inverted bands. However, intrinsic native defects in these TIs often lead to metallic bulk conductivity. The compound $Bi_{2-x}Sb_xTe_{3-y}Se_y$ (BSTS) achieves an insulating bulk by compensating the presence of donors and acceptors. One of the most intriguing transport phenomena in TIs is the quantized anomalous Hall effect, desired for devices based on magnetic topological insulators. Magnetic substitution can open a gap at the Dirac point on the gapless TSSs, which is crucial for achieving the QAH effect in a 3D TI, therefore usually ferromagnetism is introduced by magnetic substitution into TIs.
Tb has been substituted in surface dominant BSTS in order to introduce the ferromagnetism into TIs. Rare-earth elements have large magnetic moments, which can create a wider band gap on the TSS and may enhance the survival temperature of QAH insulating states. Magneto-transport studies on Tb-doped BSTS samples are not explored yet, therefore we have attempted to synthesize the single crystals of $Bi_{1.21}Tb_{0.04}Sb_{0.75}Te_{1.3}Se_{1.7}$ using the modified Bridgman method. To determine the sample's crystalline quality, phase purity, and defects, we have conducted X-ray diffraction (XRD) and high-resolution XRD (HRXRD). Energy dispersive X-ray spectroscopy and scanning electron microscopy are performed for elemental composition and surface analysis. Temperature-dependent resistivity showed a metallic nature of sample and Hall measurements reveal the n type charge carriers.

L2- 0004

Demonstration of Quantum Secure Communication between Two IoT devices using Quantum Materials & Quantum Cryptographic Technology

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Abstract

The project titled "*Demonstration of Quantum Secure Communication between Two IoT Devices Using Quantum Materials and Quantum Technology*" focuses on showcasing a novel approach to secure communication in Internet of Things (IoT) networks by leveraging the principles of quantum technology. This research aims to demonstrate how quantum materials and quantum cryptographic techniques can be used to establish a secure communication link between two IoT devices, providing unprecedented security against potential cyber threats. By utilizing quantum key distribution (QKD) and the unique properties of quantum materials, such as superposition and entanglement, the project ensures that any eavesdropping attempts during the communication process can be immediately detected and thwarted. The implementation of quantum secure communication addresses the growing concern for data security in IoT ecosystems, which are increasingly vulnerable to sophisticated attacks. The successful demonstration of this technology highlights its potential for enhancing the confidentiality and integrity of IoT communications, paving the way for future applications in critical sectors such as healthcare, defense, and smart infrastructure.

L2- 0005

Frustration and quantum fluctuations in two-chain antiferromagnetic spin ladder

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Abstract

A key challenge in low-dimensional quantum magnetism is understanding the quantum phase transitions and ground states in systems where strong quantum fluctuations suppress conventional long-range order, leading to exotic phases of matter. The Heisenberg spin ladder serves as a crucial link between one-dimensional (1D) and two-dimensional (2D) spin systems, with a valence bond solid (VBS) phase emerging under strong rung interactions and a Haldane phase for dominant leg interactions. In this study, we analyze a frustrated spin ladder model with nearest-neighbor and next-nearest-neighbor interactions, specifically for the interaction ratio $J1 : J2 : J3=2:1:1$ this model is exactly solvable, where J1 represents the rung coupling J2 is the leg interactions and J3 is the second nearest-neighbor interaction. Using triplon mean-field theory and density matrix renormalization group (DMRG) methods, we find that the ground state of the model in this parameter regime is a direct product of singlets. This phase is gapped, requiring finite energy for a spin-1 excitation stable for $J1>2J2$ at $J2=J3$. Our study provides insight into the effects of frustration and interaction strengths on the quantum phase diagram of spin ladders.

L2- 0006

Unlocking Quantum Materials: A Detailed Review of Properties and Potential

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Abstract

Quantum materials represent a rapidly evolving field in condensed matter physics, where emergent quantum phenomena arise from the collective behaviour of electrons. These materials have garnered substantial interest due to their potential to revolutionize future technologies. This review delves into four major categories of quantum materials—Weyl semimetals, superconductors, graphene, and quantum spin liquids—exploring their unique properties, underlying physics, and prospective applications in next-generation devices.

Weyl semimetals stand out for their unique topological properties, characterized by linear band crossings known as Weyl nodes. Weyl semimetals offer exciting opportunities for the development of new electronic devices, particularly in the realm of high-speed, low-energy-consumption electronics. Their ability to support dissipationless current flow under specific conditions may also have implications for quantum computing and data storage.

Superconductors, another cornerstone of quantum materials, exhibit zero electrical resistance below a critical temperature and the expulsion of magnetic fields via the Meissner effect. High-temperature superconductors have driven significant advancements in the field, with their potential to revolutionize energy transmission, magnetic levitation, and quantum computing. The challenge of understanding the mechanisms behind unconventional superconductivity remains an active area of research. However, the potential applications of these materials, such as SQUIDs and efficient quantum bits (qubits) in quantum computers, are already being explored.

Graphene, a single layer of carbon atoms arranged in a two-dimensional honeycomb lattice, has captivated researchers due to its extraordinary mechanical strength, electrical conductivity, and flexibility. The material's massless Dirac fermions enable it to exhibit a host of quantum phenomena, including the quantum Hall effect and ballistic electron transport.

Quantum spin liquids represent a more mysterious and less explored class of quantum materials, characterized by highly entangled spin states that do not exhibit long-range magnetic order, even at very low temperatures. These materials host exotic excitations, such as spinons, which behave as fractionalized particles. Quantum spin liquids have potential applications in quantum information processing, as they may serve as the basis for faulttolerant qubits in topological quantum computers.

L2-0007

Coherently Coupled Transport and Weak – antilocalization in Topological Crystalline Insulator Thin Films

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Abstract

We report low-temperature magnetotransport properties of the topological crystalline insulator (TCI) thin films of SnTe. These thin films are grown by pulsed laser deposition technique and the thickness of these thin films is kept 60nm. The temperature dependent sheet resistance of SnTe thin films shows a typical metallic behavior, followed by a sharp logarithmic upturn in the low-temperature regime (20K). This upturn in the sheet resistance (RT) is attributed to the electron-electron interaction driven upturn in the sheet resistance in the disordered electronic systems. The low temperature magnetoresistance measurements are performed on the Hall bar devices of as grown thin films. These thin films show pronounced weak-antilocalization in the low temperature regime, which is a signature of a two –dimensional transport. However, the defect generated bulk also contributes and couples with the surface transport channels, effectively making a coherently coupled transport. Our results pave a new direction towards pinning the Fermi level in SnTe class TCIs in the bulk band gap in future.

L2-0008

Structural and electronic transport properties of Zn- and Ga-doped $Bi_{2-x}Sb_xTe_{3-y}Se_y$ topological insulator single crystals

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Abstract

The structural and magnetotransport properties of $Bi_{2-x}Sb_xTe_{3-y}Se_y$ (BSTS) single crystals, and doped with Zn (BSTS:Zn) and Ga (BSTS:Ga), are systematically studied and presented here. Magnetic field-dependent Hall resistivity measurements indicate that holes are the majority carriers in these crystals. The field dependent resistivity curves, measured across various temperatures, show cusp-like behavior at low magnetic fields, which is attributed to the two-dimensional (2D) weak antilocalization (WAL) effect. The observed low-field WAL effects at low temperatures were analyzed using both 2D and three-dimensional (3D) Hikami-Larkin-Nagaoka (HLN) equations. The 2D HLN equation provided a better fit, suggesting a predominantly 2D nature of the system. The fits also revealed that the phase coherence length (l_ϕ) decreases with increasing temperature, following a $T^{-0.41}$ power law for BSTS:Zn, which points to 2D electron–electron (e–e) interactions as the key dephasing mechanism. For pristine BSTS and BSTS:Ga, $l_\phi(T)$ is consistent with a combination of 2D e–e interactions and electron-phonon (e–p) interactions. The temperature dependence of longitudinal resistance in BSTS:Ga fits a 3D Mott variable range hopping model, while the transport behavior in BSTS and BSTS:Zn is best described by a combination of 2D WAL/EEI models and 3D WAL.

M1- 0001

Characterization and Analysis of Europium Sulphide (EUS) Thin Films.

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Abstract

Europium sulphide (EuS) thin films were deposited on glass substrates using spray pyrolysis in an optimized aqueous bath. Structural analysis identified 623 K as the optimal deposition temperature for producing high-quality EuS films with excellent crystallinity, as evidenced by sharp X-ray diffraction (XRD) peaks. This temperature achieved well-crystallized films crucial for high-performance applications. Thin films were prepared from both aqueous and non-aqueous solutions containing europium (III) chloride hexahydrate (EuCl3) and thioacetamide (C2H5NS). XRD analysis confirmed the polycrystalline cubic structure of the films, with the 623 K deposition temperature yielding films with an average grain size of 16 to 35 μm and the largest crystallite sizes. Additionally, film thickness increased with temperatures above 573 K due to complete precursor decomposition. This study highlights the critical role of substrate temperature in optimizing the structural properties of EuS thin films for semiconductor applications.

Keywords: Europium sulphide (EuS), thin films, spray pyrolysis, X-ray diffraction (XRD), substrate temperature, crystallinity, semiconductor devices.

M1- 0002

Magnetic reversal and exchange bias effect in Nd-doped $SmCrO_3$

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Abstract

Nd-doped $SmCrO_3$ has garnered significant attention due to its intriguing magnetic, optical, and electronic properties, which are promising for various technological applications, including spintronics and magneto-optical devices. This study delves into the synthesis and comprehensive characterization of Nd-doped $SmCrO_3$, focusing on the impact of Nd substitution on the magnetic study. The doping of Nd-in Sm site gives rise to a zero field negative magnetization and the vanishing of glassy behaviors in $Sm_{0.9}Nd_{0.1}CrO_3$. Negative magnetization was found to be strongly dependent on the external field. The spin reorientation transition temperature and the Nèel transition temperature decrease significantly after substitution. The exchange bias effects detected in the magnetization-field isotherm curves at 5 K and 10 K confirm the strong interactions of Nd^{3+}-Cr^{3+} spins in $Sm_{0.9}Nd_{0.1}CrO_3$.

Keywords: Magnetic, Neel temperature, exchange bias.

M1- 0003

Investigating the Structural, Magnetic and Dielectric Properties of Ni^{2+} and Zr^{4+} substituted Strontium hexaferrites

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Abstract

Ni^{2+} and Zr^{4+} M type strontium hexaferrite (SrM) with chemical composition $Sr(NiZr)_xFe_{12-x}O_{19}$ (x = 0 to 0.5) were synthesized using sol gel auto combustion method. X-ray diffractogram (XRD), Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), Vibrating sample magnetometer (VSM) and dielectric measurements were used to study structural, morphological, magnetic and dielectric properties of the prepared composites. The substitution of Ni^{2+} and Zr^{4+} on the various properties of SrM has been investigated in detail. XRD results revealed the pure phase formation for the calcination temperature of 950°C. The absorption bands observed between 650 cm^{-1} to 400 cm^{-1} confirms the formation of ferrite phase. Substitution of Ni^{2+} and Zr^{4+} ions decreases the coercivity and saturation magnetization except for the concentration x = 0.1. Dielectric parameters such as dielectric constant, loss factor, AC conductivity, electric modulus and impedance were studied as a function of frequency and the result shows normal ferromagnetic behavior. At low frequencies (100 Hz to 2 MHz) the relative permittivity was constant between 100 Hz to 2 MHz.

Keywords: magnetic, hexaferrites, modulus, morphology

M1- 0004

Structural and Optical Properties of Prepared n-ZnO doped p-NiO Screen Printed Thick Films and their Applications

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Abstract

Zinc oxide (ZnO) doped Nickel oxide (NiO) thick films prepared using glass substrate by screen printing technique successfully. Synthesis of nanoparticles was confirmed using characterisation techniques, such as X-ray diffraction (XRD), scanning electron microscopy (SEM) and UV spectroscopy, FTIR, photoresponsivity. The structural properties of the prepared thick films were studied by XRD analysis. The observed prepared thick film shows polycrystalline nature of the films with a cubic structure and crystallite size found to be in the range of 18.21 to 35.44 nm. SEM analysis of prepared films enabled the conclusion that the prepared films are uniform, large crystals and heavily agglomerated particles were observed spherical in shape. Also, with increase in concentration specific surface area increases. The quantitative chemical compositions were analysed by SEM-EDS and it shows nonstoichiometric in nature. The correlation between structural and morphological properties is reported. As wt. % of ZnO additive concentration increases the absorbance of the thick film samples increases. As the size of crystallite increases the absorbance of sample also increases which is beneficial for optical sensor development.

Keywords: ZnO, NiO, Thick Films, XRD, SEM-EDS, Absorbance.

M1-0005

Synthesis and Characterization of Functionalized Carbon with DMTD Doped 6CHBT LC Media

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Abstract

We have explored the integration of functionalized CQDs with DMTD linking molecules in LC media. The carbon nanoparticles have been synthesized with the help of carbon shoot obtained from almond oil. The functionalization of CQDs has been performed with DMTD linking molecules and doped within 6CHBT LC media. In this study, our primary objective is to investigate the effect of functionalized CQDs on opto-electronic properties like band gap calculation and the behavior of LC media. The functionalized carbon NPs was linked through DMTD molecules via covalent bonding. The comprehensive characterization like FTIR (Fourier transform infrared spectroscopy), SEM (Scanning electron microscopy) and OM (Optical microscopy) confirms the functionalization of CQDs and also analyses the structural and thermal properties of doped LC molecules. Our findings underscore the potential of functionalized carbon NPs in tunning the LC media properties, paving the way for development of novel materials which tailored electro-optical properties. We have also explored HR-XRD, UV-Vis-Nir, SERS and Fluorescence data. The band gap of synthesized carbon and functionalized carbon have been calculated by UV-Vis-Nir plot.

Keywords- Carbon nanoparticles, Surface Enhanced Raman Spectroscopy (SERS), Liquid crystal media, Optical Microscopy (OM), Surface plasmon, Functionalization, CQDs etc.

M2- 0001

Decadal Analysis of Black Carbon Angstrom Exponent (470–870 nm) Over India: Spatial and Temporal Trends from 2010 to 2021

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Abstract

This study analyzes the spatial and temporal variability of the Black Carbon (BC) Angstrom Exponent (470–870 nm) over India from 2010 to 2021. The Angstrom Exponent is a critical parameter for understanding aerosol particle size distribution, with higher values indicating smaller particles. Using satellite-derived BC data, annual trends were mapped across different regions. The northern regions, particularly the Himalayas, consistently showed higher Angstrom values, reflecting the dominance of fine BC particles, likely influenced by seasonal biomass burning and anthropogenic activities. Southern and central regions exhibited increasing BC concentrations over the decade, correlating with rapid urbanization and industrial growth. Notable shifts in aerosol behavior were observed in the years 2012, 2016, and 2020, driven by changes in emission sources and meteorological factors. This study provides key insights into the regional distribution of BC aerosols, with implications for climate change, atmospheric pollution, and policy measures to mitigate BC emissions across South Asia.

N1- 0001

Bismuth and Tellurium Co-Doping: A Route to Improve Thermoelectric Efficiency in InSe Polycrystals

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Abstract

Indium selenide (InSe), a layered chalcogenide material, has gained substantial scientific interest as a thermoelectric material due to its intrinsic low thermal conductivity. However, its intrinsic carrier concentration is notably minimal (~10^{14} cm^{-3}) due to a significant bandgap of 1.3 eV. Therefore, to optimize InSe-based materials for thermoelectric applications, it is essential to increase the carrier concentration through precise doping methodologies. In this study, co-doping at both the anion and cation sites of InSe was achieved by introducing Bi to the In site and Te to the Se site. The impact of this co-doping on the thermoelectric performance of InSe-based materials was thoroughly investigated. The increase in carrier concentration due to the electron-donating nature of Bi significantly enhanced the electrical transport properties. Although there was a slight decrease in the Seebeck coefficient (S), primarily due to an increase in the effective mass (m*), the incorporation of Bi atoms resulted in a substantial improvement in the power factor (PF) across the temperature range. Among all the samples studied, $In_{0.96}Bi_{0.04}Se_{0.97}Te_{0.03}$ exhibited the highest PF throughout the temperature range. The dopants Bi/Te acted as an effective phonon scattering center, reducing lattice thermal conductivity. The synergistic effect of cation-anion co-doping resulted in a maximum ZT of ~0.13 at 630 K in the $In_{0.96}Bi_{0.04}Se_{0.97}Te_{0.03}$ sample, which is nearly 11 times higher compared to the pristine sample. Considering these findings, Bi-Te co-doped InSe emerged as an auspicious material for thermoelectric applications.

N1- 0002

Polymer Electrolytes for Improving the Performance and Safety of Lithium-Ion Batteries

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Abstract

The growing global energy demand coupled with environmental protection measures is driving the need for advanced energy storage technologies capable of storing power generated from renewable sources like wind, solar and hydropower, enabling broader integration of these sustainable energy systems. Among various energy storage systems, batteries have proven to be the most efficient. In particular, lithium-ion batteries (LIBs) have emerged as the most reliable and suitable energy storage devices due to their unique characteristics, including high energy density, high theoretical capacity, lightweight structure and longer lifespan compared to other battery technologies. However, to further enhance their energy and power densities and to address safety concerns caused by dendrite growth in the anodes, further optimization is required. Of the three key components of a battery; (i) cathode, (ii) anode and (iii) electrolyte, the electrolyte plays a critical role, significantly influencing the electrochemical performance and overall operation. Solid polymer electrolytes have attracted considerable attention in high-performance LIBs due to their improved safety, no leakage, wide electrochemical stability window, mechanical flexibility and thermal stability. This paper discusses various types of polymers such as PMMA, PEO, PAN, PVDF, PVC, PS and PC, focusing on their synthesis methods and electrochemical performance. The aim is to provide insights into their potential to further advance LIB-technology.

N1- 0003

Statistical Analysis of Air Pollutants During 2021 to 2023 Over Central Part of India. i.e., Indore and Jabalpur

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Abstract

India has been a significant contributor to human-made emissions over the past decade, driven by its swift economic and industrial development. This study analyzes nitrogen dioxide and ozone concentrations, as well as their related Air Quality Index for Jabalpur and Indore. The average concentration of NO_2 and Ozone was found in Jabalpur 35.44 µg/m³ and 41.98 µg/m³ and 52.50 µg/m³ and 44.95 µg/m³ in Indore respectively. The correlation between NO_2 and Ozone concentrations in Jabalpur and Indore was -0.24 and -0.23 indicating similar pattern. The findings highlight the variability in air quality across the central part of India, with both cities exhibiting significant fluctuations in pollutant levels and a notable correlation between NO_2 and Ozone concentrations. The study focuses on evaluating the atmospheric conditions in these metropolitan regions and investigating the chemical reactions that lead to the creation of ozone.

Keyword: - Air pollution, Surface Ozone, Nitrogen Dioxide, Ozone Formation Potential (OFP), Seasonal Decomposition

N1- 0004

Sustainable Future of Solid-State Electrolytes: A review

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Abstract

Sustainable solid-state electrolytes (SSEs) are becoming more widely acknowledged as an essential part of the development of next-generation energy storage systems, especially for integration of renewable energy sources and electric vehicle applications. SSEs provide improved performance, stability, and safety over traditional liquid electrolytes. But as the demand for green technologies increases, there is rising concern about the sustainability of these materials, both economically and environmentally. This paper examines the state of sustainable SSEs today, with a focus on the utilization of plentiful, recyclable, and ecologically friendly materials in polymer, ceramic, and composite electrolytes. It talks about trade-offs between material sustainability and electrochemical efficiency, as well as the difficulties in scaling these technologies while keeping high performance. Furthermore, the analysis highlights significant developments and trends that will probably influence the direction of sustainable SSEs in the future.

N1- 0005

Structural Study of $LiCoO_2$ Synthesized by Sol-Gel Method at Various Temperatures

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Abstract

The growing need for energy storage, driven by the shift to renewable energy, is essential for reducing environmental impact. Lithium-ion batteries (LIBs) offer high energy density and long life, making them a key technology in this transition. Their lightweight design also helps lower emissions in portable devices, contributing to a more sustainable energy future. A critical component in LIBs is the cathode material, which plays a major role in determining the battery's overall performance, capacity, and stability. Among the various cathode materials, $LiCoO_2$ is widely used due to its excellent electrochemical properties and stability. In this study, we synthesized $LiCoO_2$ using the sol-gel method at different temperatures to investigate how temperature affects its structural and morphological properties. X-ray diffraction (XRD) was conducted to confirm the phase formation and crystallinity, while Field Emission Scanning Electron Microscopy (FESEM) was employed to analyze the surface morphology and particle size. The impact of temperature on the structural characteristics of $LiCoO_2$ is reported and discussed in detail.

N1- 0005

A Solar Energy based Dryer for Environmental Sustainability, for Accelerated Drying of Vegetables

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Abstract

The use of solar energy in drying application is becoming an important and viable alternative since it decreases consumption of conventional energy by 27-80 % at an average solar collector efficiency of 40 % (Arata et al., 1993). In addition, it can easily provide low temperature requirement of heat for drying of fruits and vegetables (Mahapatra and Imre, 1990). In this view a mixed mode cabinet solar dryer of 20 Kg. capacity was designed/developed and tested at Department of Renewable Energy Engineering, CAET, NAU, Dediapada, in the present study. Mixed mode solar dryer is the combination of direct and indirect type of solar dryers in which product to be dried is heated directly by solar energy along with simultaneous heating by auxiliary air heater (Flat plate solar collector) for accelerated rate of moisture removal. Present dryer replaces the conventional energy-based dryer with solar dryer. Primary parameters considered for design of the solar dryer are Amount of moisture to be removed (Ww), Average drying rate (Wdr), The volume of air required for drying, (Va), Volume flow rate of air required (Qa), Useful heat energy required (Eu), Total collector area (Ac), Dryer dimensions, Total drying (tray) area, Number of trays and Air vent dimensions. A flat plate solar collector of dimension 2 × 1 m2 was used for auxiliary heating of the dryer. The heat absorber plate of collector was made of aluminium sheet and coated with black board paint. Top of the flat plate collector is made of single glass glazing. The collector was tilt at an angle of 23°2′ from ground surface and facing towards south. Drying cabinet with absorber tray dimension of 0.97× 0.97 m2 and height of 0.80 m was used which accommodated three perforated trays with coated black paint and made of MS angle material, to hold the products to be dried. Drying cabinet was mounted on a stand which was made of angle iron at a height of 75 cm from ground surface Drying cabinet of the solar dryer had an opening of drying chamber door from the north direction. The casing of the solar cabinet is made of galvanized iron sheet. The glass shading was placed on the top of the dryer.

N1- 0006

Self-Organized Liquid Crystals for High-Efficiency Photovoltaics

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Abstract

In the field of photovoltaics, liquid crystals (LCs) have gained significant attention as a promising invention that could lead to the development of new solar energy conversion technologies. In this study, we have explored the integration of liquid crystal materials into photovoltaic systems, which also highlight the materials' variable phases, unique optical features, and capacity to improve light absorption. Because LCs can self-organize into ordered structures, they can control light in ways that conventional solid-state materials cannot. Scientists can enhance light trapping and boost solar cell efficiency by fine-tuning the orientation and alignment of liquid crystal molecules. As recent research has shown, liquid crystals can boost the spectrum sensitivity of photovoltaic systems, especially in the visible and near-infrared range. Furthermore, the built-in adaptability of liquid crystals' natural flexibility also makes it possible to create flexible and lightweight solar panels that may be incorporated into various surfaces, such as wearable technology and building materials. Controlling the molecular structure of liquid crystals also makes it possible to design dynamic photovoltaic systems that can optimize energy harvesting by changing their characteristics in reaction to external factors. This study investigates the fundamental mechanisms of light harvesting in liquid crystal photovoltaics and explores the engineering challenges hindering their practical implementation. Liquid crystal-based photovoltaics and traditional solar technologies are compared and discussed, with an emphasis on the latter's possible benefits—such as more adaptability and lower production costs. Moreover, we have also emphasized how crucial it is to maintain multidisciplinary study to fully utilize liquid crystals' potential in the development of sustainable energy solutions, opening the door for the next generation of environmentally friendly, multifunctional, and highly efficient photovoltaic systems.

N1- 0007

Structural Study of $LiCoO_2$ Synthesized by Sol-Gel Method at Different Temperatures

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Abstract

The growing need for energy storage, driven by the shift to renewable energy, is essential for reducing environmental impact. Lithium-ion batteries (LIBs) offer high energy density and long life, making them a key technology in this transition. Their lightweight design also helps lower emissions in portable devices, contributing to a more sustainable energy future. A critical component in LIBs is the cathode material, which plays a major role in determining the battery's overall performance, capacity, and stability. Among the various cathode materials, $LiCoO_2$ is widely used due to its excellent electrochemical properties and stability. In this study, we synthesized $LiCoO_2$ using the sol-gel method at different temperatures to investigate how temperature affects its structural and morphological properties. X-ray diffraction (XRD) was conducted to confirm the phase formation and crystallinity, while Field Emission Scanning Electron Microscopy (FESEM) was employed to analyze the surface morphology and particle size. The impact of temperature on the structural characteristics of $LiCoO_2$ is reported and discussed in detail.

N1- 0008

Mössbauer Spectroscopic Study of Sub – Surface Samples of the DND#28 Well of the Jaisalmer Basin Located in Western Rajasthan, India

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Abstract

Jaisalmer Basin is a pericratonic basin which deepens to southwest and lies on northwest slope of Jaisalmer Mari basement arch. The basin is a late Paleozoic- Mesozoic basin with angle of dip 3^0 to 5^0, comprises rocks of Permian age which unconformably overlie on Proterozoic basement. In the present Mössbauer spectroscopic study carried out on the sedimentary samples of Pariwar Formation of the Danewala well DND#28 of the Jaisalmer Basin. The Iron bearing mineralogy mainly found in the Fe^{3+} in clay, Fe^{2+} in clay, Siderite and Pyrite. Presence of Fe^{3+} in clay is more favorable when the humic type of organic matter is present and presence of siderite shows the poor maturity of source rocks.

N1- 0009

A Study on Hydrobhobic Coatings for Potential Dust Mitigation and Water Savings in Solar PV Plants

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Abstract

The major large scale solar PV plants are coming up in high solar radiation areas which mainly lie in arid and semi-arid places of the world. These areas face the challenges of dust deposition and scarcity of water. The top surface of the solar PV panels is transparent for allowing the solar radiation transmittance but due to dust deposition the transmittance decreases leading to reduced efficiency and power output. For removing the dust from the surface of the solar PV panels generally water is used in the cleaning of the solar PV plants, which is another issue in water scarce regions. Present study explores both the challenges and the probable potential solutions in form of the hydrophobic coatings. This paper is divided into two main parts. First part discusses the impact of the dust deposition on the efficiency and performance of the solar PV systems. It also presents the review of the quantity of water used in the cleaning process of the solar PV systems and its influence in the water stressed regions. The second part presents the study of the different commercially available and developed hydrophobic coatings to estimate the quantity of the water required for the cleaning of the dust. The different characterization tests done on the coatings are also presented. Further, the scope for future work and challenges related to the development and use of hydrophobic coatings in the solar area are discussed.

N1- 0010

Optimizing Waste Floral Foam Derived Nanoporous Activated Carbon for Efficient CO_2 Capture: An Investigation on the Property-Performance Correlation

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Abstract

The optimal CO_2 capture requires the engineering of a low-cost, high-efficiency adsorbent. Herein, the upcycling of waste floral foam into chemically activated nanoporous carbon (CANC) is reported. The implications of the impregnation ratio of KOH on the porosity, surface functionality of CANC, and its role in CO_2 capture are examined and discussed. The optimized sample, CANC-2, with a large ultra-micropore volume and higher oxygen and nitrogen content, demonstrates 3.71 mmol/g CO_2 capture capacity at 15 ^oC and 1 atm. The framework provided here emphasizes the property-performance correlation while offering a technique for tuning the attributes of nanoporous carbon that are favorable for CO_2 capture.

O1- 0001

Investigation of Functional Group, Optical and Structural Characteristics of Doped and Pure Glycine $LiNO_3$ Crystals

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Abstract

Second Harmonic Generation (SHG) from the Centro-symmetric Glycine crystals in its pure form show a photo-type of waves on resistance from the guest molecule. Such Non-Linear Optical (NLO) materials have potential application in Second Harmonic Generation. An excellent optically transparent single crystal of Glycine in the presence of fractional amount of Lithium Nitrate, Potassium Nitrate and Sodium Nitrate are grown in a solution by slow evaporation method which have good non-linear optical (NLO) behavior. Powder X-ray diffraction spectrums were recorded using a diffractometer with Cu-Kα radiation, scanning in the 85 degree range for 8 minutes. The paper studies exhibit the powder XRD pattern of the grown crystals after calculating lattice parameter values, particle size, dislocation density, strain values etc. the X-ray Diffraction studies shows that the crystalline perfection of grown crystals is extremely good with no internal structural grain boundaries. In order to investigate structural phase, presence of different chemical bonds or additional elemental group etc. within grown crystals, they were examined by the spectrum of Fourier Transform Infrared (FTIR) Spectroscopy. Assigned vibration of various chemical bond groups were identified and confirmed by this investigation. Optical Characteristics of Doped and Pure Glycine $LiNO_3$ Crystals were carried out by visible and ultraviolet (UV) spectra and bandgap (E_g) of the synthesized sample were calculated. For a nonlinear application, it was determined that the optical transparency and cutoff wavelength needed to be equals to 300 nm. For $NaNO_3$ with concentration of 20% and 60% doping, the band gap was found as 6.07 eV and 5.84 eV respectively. For KNO_3 doping with concentrations of 20% and 60%, the energy band gap was found to be 6.21 eV and 5.88 eV respectively.

O1- 0002

Perovskite solar cells devoid of lead: stability assessment

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Abstract

Photovoltaic technology, which directly converts solar energy into electricity, has become more and more popular in response to the growing demand for clean and sustainable energy sources. Over the past few years, their power conversion efficiency has rapidly increased from 3.8% to 25.5%. The chemical formula of perovskite solar cell is ABX3, where A stands for both organic and inorganic cations, B for the metal cation (Pb2+), and X for halogen anion. Since lead (Pb) is toxic in nature. A few review articles focus on less toxic or non-toxic ions, their properties, sustainability, and difficulties associated with replacing lead with metals like Sn, Ge, Bi, Ti, Ag, and Cu. Tin has shown to be a viable substitute for lead (Pb) in terms of reaching benchmark performance. Increasing the visibility of these Sn PSCs is essential to advancing low Pb or Pb-free PSCs in terms of both research and commercialization. Low stability of perovskite solar cells is one of the primary barriers preventing them from becoming commercially viable. These viewpoints are beneficial for perovskite solar cells with a tin based commercialization. This review article, will focus on tin-based PSCs (theoretical and experimental results), along with use of different charge transport layers which are helping in the stabilization of the device.

O1- 0003

Cleaning and early oxidation of W(110)

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Abstract

One of the most popular substrates for thin film formation is the densely packed (110) surface of tungsten because it has the highest melting point of any metal (3683 K) and is brittle and hard, especially when impurities like carbon and oxygen are present. In comparison to other metal substrates like Ag(001), Ag(111), the cleaning of W(110) is more challenging since it contains carbon and oxygen. Carbon from the bulk is segregated onto the crystal's surface by annealing it at a very high temperature. This is typically followed by oxygen annealing and flash at high temperature that extracts carbon as CO and CO_2. However, tungsten oxide production was seen during cleaning, as evidenced by the low energy electron diffraction (LEED) pattern resembling twin domain tungsten oxide (WO_2). The domain is extremely similar to the (1×1)×12 LEED pattern and may be described in matrix notation $\begin{bmatrix} 0 & 9 \\ -2 & 5 \end{bmatrix}$. Oxygen annealing temperature, partial pressure, flash temperature, and duration can all have a significant impact on how the cleaning process turns out in the end. By oxygen annealing at five different pressures, ranging from 1×10^{-6} mbar to 7×10^{-8} mbar, for thirty minutes at a time, a final clean surface was achieved. The flashing process lasted just 5–10 seconds at a temperature higher than 2373 K.

O1- 0004

Molybdenum removal from aqueous solution by Surfactant Modified Mordenite (SMM)

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Abstract

Surfactant modified mordenite (SMM) was used as an adsorptive material to treat molybdenum containing aqueous solution. The solution pH was adjusted 7 to study the influence of pH on molybdenum removal. The aqueous molybdenum uses on various pH ranging from 1 to 9 and SMM to molybdenum ratio in different concentrations on temperature ranging from 15^0C to 35^0C in varying contact time from 1 to 24 hrs to study the removal efficiency. The results show that the molybdenum removal mechanism is a surface adsorption process that could be fit by a Freundlich adsorption isotherm. The solution pH controls the process and the optimum pH is 7 and equilibration time of 7 hrs confirmed by the kinetic study. This process can be combined with conventional water treatment plant to protect drinking water safety when the raw water contains trace molybdenum pollution.

Keywords: Surfactant modified mordenite (SMM), molybdenum, and adsorption

O1- 0005

Structural electronic and spectroscopic properties of Eu^{3+} doped $Ca_3Al(PO_4)_3$ phosphor

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Abstract

In this paper, Eu^{3+}-doped $Ca_3Al(PO_4)_3$ phosphor is successfully synthesized by using co-precipitation method. The structure, Rietveld analysis and photoluminescence properties are investigated. XRD analysis confirms the phase formation of the phosphate-based compound, revealing a cubic structure with space group I43d and was verified by Rietveld analysis. The prominent emission peaks at 615 and along with 657 nm observed in the orange-red region, primarily attributed to the dominant forced electric dipole transition from the $^5D_0 \rightarrow {}^7F_{2,3}$ electronic state. The yellow emissions, peaking at 580 and 591nm are linked to the dominant magnetic dipole transition from the $^5D_0 \rightarrow {}^7F_j$ (j = 0, 1). The study also explores the concentration quenching mechanism, indicating that multipolar interaction is responsible for the quenching of PL intensity. The asymmetric ratio (R_{21}) of the PL spectrum of Eu^{3+} is calculated confirming the occupancy of Eu^{3+} ions in the normal site within the host matrix. The Judd-Ofelt analysis parameters are also examined. Moreover, this novel phosphate phosphor has a potential for pc-converted LEDs using N-UV chips for solid-state lighting applications.

Keywords: Luminescence, Structure refinement, Eu^{3+} emission, Judd-Ofelt analysis

O1- 0006

Role of site symmetry on luminescence spectrum of Ce^{3+} and Eu^{2+} doped aluminate based phosphors

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Abstract

The role of site symmetry is an important parameter in rare earth doped phosphors to analyze the optical behaviour leading their mankind applications. The site symmetry exhibits in various coordination numbers within the host matrix. Predominantly, site symmetry affects the broad PL emission that arises from Ce^{3+} and Eu^{2+} in aluminate based phosphors. The Ce^{3+} and Eu^{2+} ions provided the broad band emission spans over the UV to red region of spectrum due to $4f \rightarrow 5d$ transition normally of spin-orbit coupling. The 5d energy level of Ce^{3+} and Eu^{2+} ions is certainly affected by the crystal field splitting within the host matrix. The alteration in the site symmetry can be achieved by using appropriate synthesis methods and alteration of temperature. The modification of site symmetry leads to blue-red shift in the PL spectrum of Ce^{3+} and Eu^{2+} doped aluminate based phosphors. The site symmetry effect is a key parameter in achieving the broad band emission in a single host. In this paper, few reports of Eu and Ce doped $BaAl_2O_4$, $ZnAl_2O_4$, $SrAl_2O_4$ and $Y_3Al_5O_{12}$ phosphors are discussed and presented.

Keywords: Luminescence, Aluminate phosphor, broadband phosphor

O1- 0007

Recent developments and challenges in Green machining- A review

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Abstract

Green machining is a rapidly emerging field aimed at minimizing the environmental impact of machining processes while maintaining or enhancing economic efficiency. Traditional machining operations often rely on cutting fluids to reduce friction and heat during cutting, but these fluids can have significant negative effects on both the environment and human health. As industries strive for high productivity, zero-defect quality, improved efficiency, and time savings, these advancements have often come at the cost of environmental degradation. In response, sustainable manufacturing practices are gaining global importance, incorporating various strategies to conserve natural resources and protect the environment. Machining, a critical segment of the manufacturing sector, produces engineered parts and components for both capital and consumer goods through processes that typically leave a large environmental footprint. This has driven the development of green machining techniques, including hybrid machining, eco-friendly lubrication methods, dry-cutting, energy-efficient machining and assisted machining processes. This paper explores several of these green machining techniques, developed for both conventional and non-conventional machining, aimed at achieving a cleaner, greener, and safer manufactring environment.
The paper reviews the environmental and economic impacts of cutting fluids and proposes alternatives to traditional methods. Additionally, it discusses recent challenges and innovations in green machining, highlighting the potential benefits for both the environment and the economy. It is hoped that these techniques will play a key role in the success of future industrial revolutions.

O1- 0008

Comparative Analysis of Different Versions of 'Area Method' in Thermoluminescence Glow Curve Analysis Considering Temperature DependentFrequency Factor

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Abstract

Area Method is one of the widely used techniques in thermoluminescence (TL) glow curve analysis to extract different trapping parameters of the phosphor. The Area method utilizes different portions of the glow curve, provides reliable and precise values of trapping parameters. Several versions of the area method have been developed, such as those by Kirsh, Rasheedy, and the Three-Point Area (TPA) method. In this study, we have used Kirsh method, Rasheedy method and TPA method on TL glow curves simulated in General Order Kinetics (GOK), One Trap One Recombination center (OTOR) and Interactive Multi-Trap System (IMTS) models considering temperature-dependent frequency factor (TDFF) under quasi-equilibrium approximations in linear heating scheme. The frequency factor (s) in thermoluminescent materials varies with temperature and can be represented as $s(T) = s_0 T^a$, where $-2 \leq a \leq 2$. However, TL glow curve analysis is often performed under the assumption that the frequency factor is temperature independent due to the challenges in estimating the value of a. This assumption can lead to inaccuracies when determining TL parameters in a material. Therefore, it is crucial to thoroughly investigate the impact of temperature-dependent frequency factor (TDFF) on TL analysis. Activation energy (E) and kinetic order (b) are estimated for different values of 'a' using the above mentioned models and a comparative study is reported. The present study is also applied to some experimental TL peaks and the limitations and future scope are also discussed.

O1- 0009

Transition Metal Oxide (CuO) as an Electrode Material for Energystorage Applications

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Abstract

The use of nonrenewable fossil fuels for energy has increased over the past few decades, posing a serious threat to human life. Therefore, it is imperative to develop inexpensive, environmentally safe, and dependable renewable energy storage solutions. Transition metal oxides (TMOs), one of the discovered active materials, have drawn interest as electrode options for supercapacitors (SCs) because of their outstanding redox chemistry, multivalence states, high theoretical capacity, and reasonable cost. Here, CuO has been prepared by using chemical route for their application as electrode material in supercapacitors. The prepared material characterized structurally with the help of X-ray diffraction (XRD) and optically with the help of UV-Vis spectroscopy and photoluminescence (PL). Energy band gap of synthesized material has been calculated by using Tauc plot. The electrochemical performance of the prepared material has been studied in 1M Alkali aqueous electrolyte (KOH) by using cyclic voltammetry, galvanostatic charge-discharge methods and electrical impedance spectroscopy. We get the different values of specific capacitance at different scan rates (5, 25 ,50 and 100 mVs-1) and different current densities. The prepared CuO material shows a maximum specific capacitance at 5 mVs -*1* scan rate *Synthesis of Copper Oxide (CuO) nanoparticles*

O1- 0010

Study of Growth of Rare-Earth doped Bismuth

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Abstract

Bismuth has low melting point and can grow in single crystal form easily. Bismuth shows high Magneto-resistance and topological properties. We can enhance its properties by magnetic doping. Here we choose rare earth (RE) elements (Gd, Nd and Eu) into Bismuth. Rare earth elements can break the time reversal symmetry and can leads to anomalous quantum hall effect. We attempted to synthesis the rare earth doped bismuth crystal by using modified Bridgman technique. X-Ray diffraction (XRD) measurements performed on prepared samples shows RE went into the lattice of Bismuth as evident from the shift in lattice planes. Energy dispersive X-Ray analysis (EDAX) also confirmed the presence of doped elements along oxygen due to oxidizing nature of RE. Electrical and magnetic measurement investigation is underway to explore the topological effects.

O1- 0011

Characterization of Gel Grown Pure SrT and Mixed Sr-Mg-Zn Ternary Levo-tartrate Crystals

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Abstract

In the present investigation, single crystals of pure strontium tartrate (ST) and strontium-magnesium-zinc ternary levo-tartrate (SMZT) crystals have been grown by single diffusion gel growth technique in silica hydrogel medium at room temperature. The obtained pure ST and SMZT crystals were opaque having dimensions of 10x8x6 mm^3 and 7x3x2 mm^3 respectively. The presence of expected elements in crystals was confirmed by carrying out EDAX spectrum analysis The scanned images show these crystals to be grown by layer deposition. The thermal stability of the crystals was studied by thermogravimetry and by using the standard Broido relation, the activation energy and various kinetic parameters such as change in entropy, enthalpy, and Gibbs free energy for all the crystals were obtained and studied. TG curves obtained for pure ST and SMZT crystals showed different temperatures for each of them indicating different degrees of thermal stability.

Keywords: Gel growth, PXRD, EDAX, TGA, FTIR, SEM

O1- 0012

Engineering the optoelectronic properties in NiO Thin Films through Zinc Substitution for Photo-detector Applications

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Abstract

Nickel oxide (NiO) has recently attracted significant interest in optoelectronics due to its advantageous properties, including p-type conductivity, chemical stability, and a simple cubic structure conducive to easy elemental substitution. Zinc oxide (ZnO), another widely studied material, is notable for its n-type conductivity, wide bandgap, fast photoresponse, and natural abundance. In this study, we fabricated spray-deposited NiO thin films with systematic incorporation of zinc into the NiO lattice, examining the resulting structural and optical changes. The addition of Zn induced a modification in grain structure, while optical analysis revealed increased absorbance and a bandgap reduction from 3.52 eV to 3.20 eV. Furthermore, with more than 60% substitution of Ni with Zn, the films exhibited a transition from p-type to n-type conductivity with an increase in resistivity from 2.7k to 5.7kΩcm . The photoresponse was also enhanced by Zn alloying, indicating the potential of these films for photodetector applications.

O1- 0013

Unveiling the Potential of Tungsten-Lithium-Strontium-Bismuth-Borate Glasses

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Abstract

Glasses based on lithium-strontium-bismuth-borate incorporating tungsten ions exhibit distinctive synthesis, thermal, structural and physical properties. These glasses are effectively fabricated utilizing melt-quenching techniques, facilitating the integration of tungsten ions. The inclusion of tungsten substantially impacts the thermal properties and physical characteristics, thereby enhancing the overall glass performance. X-ray diffraction analysis confirmed the amorphous nature of the prepared glasses. Additionally, physical and differential thermal analyses indicated increasing density, Refractive index and glass transition temperature following the incorporation of tungsten. The glasses that were prepared exhibit an increase in basicity when there is a low level of electron donation, which in turn leads to higher chemical durability. Furthermore, the polarizability of the oxide ion is enhanced as the concentration of tungsten increases. This enhancement results in a greater formation of non-bridging oxygen (NBO) bonds, contributing to the overall properties of the glasses. The FTIR analysis indicates that the glass composition's OH bond is absent at 3300 cm^{-1}. This absence is expected to enhance the luminescence properties of the glass by preventing quenching effects. Furthermore, the FTIR analysis also reveals the presence of major borate and metal ions bonds in the composition. The differential scanning calorimetry (DSC) analysis indicates that the glass transition temperature falls between 410 to 430 degrees Celsius.

O1- 0014

Detection of Chlorine and Fluorine in water using Functionalized Carbon nanotubes

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Abstract

The presence of ions in water plays an important role which dramatically affects the properties of water. The presence of ions and their concentrations have been considered an important factor for water quality assessment. Due to their significant effects on the hardness, taste and suitability of water for a wide range of applications. The ions are present in the form of cations and anions, and their presence are essential up to their permissible limit. In this study, the 5 MHz AT-cut quartz crystal has been functionalized with octadecyl amine carbon nanotubes (ODA-SWCNTs) using spin coating technique to monitor the free chlorine and fluorine in aqueous medium at ppb level. The resonance frequency of quartz crystal is ultrasensitive to the mass changes on its surface. The solid powder of chloride and fluoride are decomposed into the water and changed into the chlorine and fluorine. Due to adsorption of free chlorine and fluorine onto the functionalized quartz surface, its resonance frequency is decreases. The adsorbed quantity of anionic species was estimated through the decreased frequency of crystal. The resonance frequency of the functionalized crystal was continuous monitoring while the interaction of anionic species with sensing layer. The lowest detection limit of fluorine, chlorine was found to be 2 and 0.5 ppb, respectively. The natural polymer and cheap beeswax used to provide the stability to ODASWCNTs in aqueous medium which increases the sensitivity and reproducibility of ODASWCNTs sensing layer.

Keywords: Piezoelectric, Quartz crystal, Chlorine, Fluorine, resonance frequency.

O1- 0015

Investigation of Structural and Optical properties of Yttrium Aluminium Borate (YAB) Synthesized via Solid-State Reaction method

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Abstract

Yttrium aluminium borate ($YAl_3(BO_3)_4$), commonly referred to as YAB, is a nonlinear optical material that has demonstrated exceptional performance in both display and lighting applications. It exhibits distinctive physical and chemical properties compared to other borates. Notably, YAB features a broad optical transparency extending into the short UV range, a high optical damage threshold, excellent thermal and chemical stability, a high decomposition temperature and is non-hygroscopic. These attributes make YAB a unique candidate for achieving superior optical properties. Consequently, the present work focuses on synthesizing polycrystalline YAB and investigating its structural, optical, and magnetic properties.

In the present study, Yttrium Aluminium Borate (YAB) was synthesized using the solid-state reaction method. The structural properties of the material were analyzed through X-ray diffraction (XRD), confirming the formation of a single-phase YAB without any impurity phases. Morphological characterization was conducted using Scanning Electron Microscopy (SEM), showing a rod like shape of the particles. Energy Dispersive X-ray Spectroscopy (EDAX) was employed for elemental analysis, with results confirming that the elemental composition aligns with the stoichiometric ratio of YAB. Additionally, Fourier Transform Infrared Spectroscopy (FTIR) was performed. The bands in FTIR at 792, 725, and 684 cm^{-1} confirm Y–O bond stretching, indicating the presence of metal-oxygen bonds. Also, the peaks at 563 cm^{-1} and 439 cm^{-1} correspond to Al - O vibrations associated with the octahedral sites in the garnet structure. These results confirm the formation of yttrium aluminium garnet. Further emission studies will be conducted to explore the potential applications of YAB. The prepared YAB may be a potential candidate for LED and other related applications.

Keywords: YAB phosphors, XRD, FTIR and Optical studies.

O1- 0016

Low Effective Mass and Anisotropy of Electron in n-Type Tin Europium Telluride

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Abstract

In this study, we investigate the properties of n-$Sn_{1-x}Eu_xTe$, focusing on band dispersion and effective mass, within the context of the $\vec{k}\cdot\vec{\pi}$ model. The calculations are performed at T=300 K, using a simulated energy band gap that varies with the concentration of Europium impurity x. The energy dispersion demonstrates non-parabolic behavior, which follows a 4th-order polynomial in k. we derive the effective mass equation from Green's function perturbation method in the presence of spin-orbit interaction and external magnetic field. The Peierls' phase factor is used to preserve translational symmetry of the Green's function disrupted by the presence of magnetic field. We conduct a thorough investigation of the effective mass and its anisotropy before and after the band inversion point at x=0.020, taking into account the experimentally simulated band gap. Additionally, we examine the behavior of the effective mass of n-$Sn_{1-x}Eu_xTe$ with respect to the variation of temperature by considering the expression of simulated energy band gap from optical absorption spectra from the experiment. Our results show exceptionally low values for the effective mass, specifically m=0.005 m_0 at x=0.018 in the concentration range $0.01x10^{19}cm^{-3}$ to $0.1x10^{19}cm^{-3}$, where m_0 denotes the free electron mass, for n-$Sn_{1-x}Eu_xTe$. Low effective mass holds significant potential for spin-based devices like spin-Field Effect Transistors, as it results in higher carrier mobility, which is highly desirable for spintronics applications.

Keywords: $\vec{k}.\vec{\pi}$ method, spin-orbit interaction, 6-Level band structure, Effective mass, s/p-f hybridization

O1- 0017

Volatile Organic Compounds as Biomarkers: Innovations in Cancer Biosensors for Early Diagnosis

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Abstract

Malignant tissues emitting volatile organic compounds (VOCs) are one unique and non-invasive way to diagnose cancer early. Some cancers release unique volatile organic compounds (VOCs), such as those of the breast, lung, and colon. Among the bodily fluids that emit these metabolic byproducts are breath, urine, and sweat. Discovering volatile organic compound (VOC) profiles specific to cancer has attracted a lot of attention as a possible diagnostic tool, especially for cancers that are challenging for traditional methods to detect in their early stages. Patients with breast cancer have been shown to emit certain volatile organic compounds (VOCs), including alcohols, hydrocarbons, and aldehydes. Similarly, lung cancer biomarkers, like alkanes and benzene derivatives, can be found in exhaled air and offer a non-invasive diagnostic technique. Patients with colon cancer also have unique volatile organic compound (VOC) fingerprints in their breath and faeces, such as esters and short-chain fatty acids. Biosensors based on nanotechnology, like those that use graphene, carbon nanotubes, or metal oxide semiconductors, have been created to detect volatile organic compounds (VOCs) with great specificity and sensitivity. When volatile organic compounds (VOCs) are present, these sensors pick up on changes in electrical, optical, or electrochemical characteristics. VOC detection systems can distinguish between patterns specific to cancer and normal biological fluctuations when used in conjunction with machine learning algorithms, improving the accuracy of the diagnosis.With additional development and validation, VOC-based biosensors could transform cancer diagnostics by offering quick, affordable, and non-invasive screening methods, greatly improving patient outcomes through early intervention. Biosensors based on volatile organic compounds (VOCs) present a promising approach for early cancer detection, especially for breast, lung, and colon cancers.

O1- 0018

Solvent Effects on the UV-Visible Absorption & Emission of 1,3,5-triphenylbenzene (TPB)

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Abstract

1,3,5-triphenylbenzene (TPB) is an organic molecular semiconductor generally used to enhance the charge transport of the devices for some time now. TDAPA is dissolved in various Polar and Non-polar solvents like DMF, Acetone, Acetonitrile, Ethanol, Methanol, Toluene and Chloroform. Absorption spectrum of solution is recorded using UV-Vis spectroscopy and absorption peak for different solvents were observed in UV and Near-UV region. PL study and Pl Excitation study is also carried out for these solvents. Results for absorption and photoluminescence show some interesting phenomenon of Stokes' shift. The colour coordinates for respective emission are represented by CIE 1931. The study is successfully carried out for better understanding of effect of these solvents on the optical properties of TPA.

O1- 0019

Degradation of methylene blue dye through Hydrothermally synthesized PPy/ Fe_2O_3/ZnO nano-composites

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Abstract

In present scenario, the polymer-based metal oxides nano-composites have multiple scope for today researcher because of their reliability, cost effectiveness and long life for user applications. In present work the Fe_2O_3/ZnO nano-composites were synthesized by the enhanced hydrothermal technique. The oxidative polymerization of pyrrole used to prepare the polypyrrole (PPy) solution. The in-situ method was employed to produce mixed metal oxides/PPy nano-composites. The structural, optical and morphological characteristics of polymeric nano-composites were examined. The photo-sensitivity of PPy/ Fe_2O_3/ZnO nano-composites was investigated for the degradation of methylene blue dye under visible light of 100Watt Bulb. The fluctuations in pH and colour were continually monitored across the degradation period of the dye. The pH rises and the colour diminishes as the photo-degradation of the dye progresses over time. The optical band gap of metal oxide nano-composites, poly-pyrrole (PPy), and PPy/metal oxide nano-composites was examined through UV-Vis-IR spectroscopy and Tauc plots. The photo-generative degradation of methylene blue adheres to pseudo first-order kinetics, with a rate constant of 0.0694 min−1. The metal oxide/PPy nano-composites (90 ppm) destroy 82% of methylene blue dye after 90 minutes of continues exposure of white (visible) light. The magnetic characteristics exhibit a significant level of magnetization residual/retention in polymeric coated nano-composites. The metal oxide/PPy nano-composites exhibit excellent photo-catalytic, optical and magnetic capabilities, hence serving as sophisticated multi-functional nanomaterials for diverse applications.

Keywords: PPy/ Fe_2O_3/ZnO nano-composites, XRD, FTIR, UV-Vis-IR spectroscopy & VSM tools.

O1- 0020

Tuning the Structural and Optical Properties of the Mo and W Oxide Nanostructured Thin Films

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Abstract

In this work, we explore the tuning of structural and optical properties of molybdenum (Mo) and tungsten (W) oxide nanostructured thin films through controlled variation of process parameters. By systematically adjusting these parameters, we observed significant changes in the morphology of the films, as characterized by Scanning Electron Microscopy (SEM). The films displayed distinct structural modifications. In addition to the structural analysis, UV-Vis spectroscopy was employed to investigate the optical properties of the thin films, revealing notable shifts in the diffused reflectance. These shifts were strongly correlated with the composition and morphology of the films, providing insights into the relationship between structural tuning and optical behavior. Our findings demonstrate that precise control over the process parameters can effectively tailor the structural and optical characteristics of Mo and W oxide nanostructured thin films, offering potential for their use in advanced optical applications. This study highlights the significance of material composition and fabrication techniques in optimizing the functional properties of oxide-based nanostructures.

O1- 0021

Polyaniline-Cadmium ferrite: nanostructured composite for resistive type humidity sensor at room temperature

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Abstract

In the present work, we have fabricated polyaniline-cadmium ferrite (PANI-$CdFe_2O_4$) nanostructred composite as a resistive type of humidity sensor at room temperature. The PANI and its composite prepared by chemical in-situ polymerization method. The prepared composites were subjected for structural and surface morphology characterizations using FT-IR, XRD, SEM and TEM techniques. The comparative XRD and FT-IR analysis confirmed $CdFe_2O_4$ embedded in PANI matrix in mutual interfacial interaction. The nanostructure of the composite was confirmed by TEM image. A simple Humidity sensor operable at room temperature, exclusively based on spin coated PANI-$CdFe_2O_4$ nanocomposite was fabricated with a maximum sensing response of 92% at 95% RH. The response and recovery time of the sensor were 40s and 60s respectively and was stable over a period of one month with a small degradation of 6%. The sensing mechanism is discussed with three successive steps of chemisorptions, physisorption, and condensation process at the interface of PANI and $CdFe_2O_4$.

Key words: Polyaniline, Cadmium Ferrite, Humidity, Sensing response, Stability, Hysteresis

O2- 0001

Controlled Higher-Order Antibunching of Light in Mltiphoton -Photon Interaction Process

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Abstract

We investigate the controlled of higher-order photon antibunching in three and four-photon absorption processes through multiphoton-photon interactions. By solving the generalized interaction Hamiltonian for various specific cases in the Heisenberg picture and employing the short-time approximation technique .we investigated the possibility of observing antibunching we found that antibunching depends on Coupling between field modes, Short-time interaction and Photon number Our results show that controlled fift--order antbunching is more pronounced, while antibunching is absent in Stokes and signal modes. Therefore, we conclude that controlled higher-order multiphoton absorption techniques are optimal for producing antibunched light.

O2- 0002

An Enhanced Simulative Study on SWIRGs of $In_{0.68}Al_{0.08}Ga_{0.24}As$/InP Lasing Nanoscale Heterostructure

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Abstract

The foremost emphasis of this foundational research letter has been given on analytical investigation of an enhanced simulative study on shortwave infrared gains (SWIRGs) of $In_{0.68}Al_{0.08}Ga_{0.24}As$/InP lasing nanoscale heterostructure for fiber optic cable communication applications under transverse electric and magnetic bi-modes at 300K. In the starting of this work, taking into account recent and emerging computational technology, an enhanced and improved effective mass theory for single and multi sub-bands has been utilized to enumerate the appropriate SWIR gain parameters as well as electrons-holes (Es-Hs) levels of quasi Fermi energies. Under advanced simulation, first of all, the salient computational performances of Es-Hs levels of quasi Fermi sub-band energies versus injected carriers (10^{18} cm^{-3}) at 300K have been analyzed simulatively. Next, electric and magnetic transverse bi-modes induced several spectral performances of SWIR-gain with wavelengths of photons have also been investigated analytically. In spite of this, the prominent performances of SWIR-differential gain in ($10^{-16}cm^2$) with injected carriers (in 10^{18} cm^{-3}) under transverse electric and magnetic bi-modes at 300K have been analyzed dominantly. Throughout the results, the peak intensities of SWIR-gain are achieved at wavelengths 1330 nm and 1550 nm corresponding to two crests of SWIR-spectra respectively under transverse bi-modes. Consequently, this emitted SWIR light gain by $In_{0.68}Al_{0.08}Ga_{0.24}As$/InP heterogeneous nanostructure of wavelengths ~ 1330 nm and 1550 nm can be substantially utilized in the applications of fiber optic cable communications in the transmission of SWIR-signals through the modern process of total internal reflection with minimal attenuations of SWIR-signals (in dB × km^{-1}) owing to lowest fiber dispersions and fiber absorptions.

Keywords: Es-Hs quasi Fermi sub-band energy levels, SWIR-gain, SWIR-differential gain, SWIR-loss, Transverse bi-modes, $In_{0.68}Al_{0.08}Ga_{0.24}As$ and InP.

O2- 0003

A review on Role of Image processing algorithms in Dynamic speckle imaging analysis and their applications

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Abstract

Laser speckle technique has been considered as a new growing emerging technique which can be applied in various field including agricultural, medical and industrial applications. In this technique, speckle image is captured and then analyzed with different image processing algorithms such as Time history of speckle pattern(THSP), Inertia moment (IM), Generalized difference (GD), Fujii and many existing methods. In the present paper, it has been shown that how a change in parameters can change the result of existing methods with more significant result in both qualitative and quantitative analysis. Results of existing and proposed algorithm in different application is shown and compared. It is concluded that proposed algorithm can be applied for more significant results in many applications.

O2- 0004

Assessment of Honey Using Spatially Filtered He-Ne Laser under Linear and Circular Polarization via Image Processing and Scattering

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Abstract

A 10 mW He-Ne laser beam undergoes polarization using a polarizer and a quarter-wave plate, generating linear and circularly polarized light. The beam is spatially filtered for optimization and directed through a diluted honey sample within a quartz cuvette, facilitating interaction that induces light scattering. Scattered light phenomena were captured using a Charge-Coupled Device (CCD) camera set to record from both polarization modes. These images underwent digital image processing to analyze six distinct features and six textures. The experimental procedure was replicated three times for each polarization state, resulting in six comprehensive data sets. Imaging occurred at sequential time intervals—2, 4, 6, and 8 minutes after sample introduction—with a temporal resolution of 108 images captured consecutively at 10 frames per second. This enables comprehensive temporal analysis of sample behavior under varying polarization conditions. To enhance reliability, averaged data from all recordings at each time interval for both polarizations is utilized. Significant percentage changes between scattered images of polarized light types are observed: variance (73%), angular second moment (35%), maximum probability (29%), mean (25%), inertia moment (132%), and absolute value difference (74%). Qualitative assessments using a Co-occurrence matrix (COM) image and Surf image analysis provided marked differentiation between scattered light images under both polarization states. The experiment effectively illustrated that polarization-dependent light scattering, integrated with image processing, provides notable discrepancies in the interaction dynamics of linearly versus circularly polarized light with honey.

O2- 0005

Band-edge mode triggered Enhanced Light-matter Interaction in a Perovskite Nanocrystals Embedded Polymer Bragg Reflector

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Abstract

Enhanced light-matter interactions are crucial in achieving advancements in various fields such as biomedical, imaging, communication, photovoltaics, optoelectronics etc. In this work, we focus on the nonlinear optical (NLO) activities of perovskite nanocrystals (NCs) when coupled with slow-photon modes in a bragg reflector. The perovskite $CsPbBr_3$ NCs are synthesized via ultrasonication method and for the fabrication of solution-processed bragg reflector, spin coating method was used. Nonlinear absorption (NLA) measurements on the samples are done using open Z-scan method and the results reveals an enhanced NLA activity in NCs in bragg reflector compared to the bare NC film. The enhanced NLA response of the perovskite NCs with bragg reflector can be imputed to the stronger light-matter interaction happened due to the reduction in light velocity at the band-gap edge of the bragg reflector structure.

O2- 0006

Assessing Water Quality Using the Normalized Difference Water Index (NDWI): A Remote Sensing Approach with Satellite Imagery."

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Abstract

The Normalized Difference Water Index (NDWI) is a widely utilized remote sensing technique for detecting and monitoring surface water bodies, as well as assessing various water quality parameters such as turbidity, suspended sediments, chlorophyll-a, and total dissolved solids. This study explores the application of NDWI across diverse hydrological settings, emphasizing its ability to delineate water features by leveraging the differential reflectance in the green and near-infrared (NIR) spectral bands. NDWI's strength lies in its capacity to enhance the contrast between water and non-water elements.

Utilizing high-resolution satellite imagery, including data from sensors like Landsat and Sentinel this paper demonstrates NDWI's versatility in monitoring both small and large water bodies. Through case studies ranging from urban reservoirs to natural lakes, NDWI's efficacy in tracking water extent changes, seasonal variations, and the impacts of anthropogenic activities is highlighted. environments like turbid or mixed-use water systems.

The study also evaluates the correlation between NDWI and critical water quality indicators, validated through in-situ measurements and ground-truth data. Results show a strong relationship between NDWI-derived data and water quality parameters, confirming its utility in large-scale, real-time water monitoring. The integration of NDWI with other spectral indices and machine learning techniques is explored to improve water detection and quality predictions. This paper touches on the broader applications of NDWI, such as its role in supporting sustainable water resource management in the face of global water scarcity challenges.

O2- 0007

The impressive nonlinear optical properties of Copper@Graphite nanoparticles synthesized by laser ablation in benzene derivative solvents

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Abstract

In this paper, we investigate the enhancement of optical nonlinearity by surface passivation of copper with graphite. Copper, known for its excellent electrical conductivity, finds extensive applications in various fields, including electronics, telecommunications, and energy. However, its optical properties, particularly its nonlinear response, remain relatively unexplored. Surface passivation with graphite offers a promising approach to modulate and enhance copper's optical nonlinearity, thereby opening new avenues for advanced photonics and optoelectronic applications. The samples were prepared through pulsed laser ablation experiments involving a copper target immersed in different solvents. The formation of Cu@graphite core-shell nanostructures was confirmed by using UV-visible spectroscopy. By employing a Z-scan setup, the optical limiting characteristics of the Cu@graphite core-shell structures were investigated, revealing that the inclusion of graphite significantly boosts the optical nonlinearity and optical limiting properties of copper. This discovery positions these structures as promising candidates for applications in laser safety. In summary, this study sheds light on the potential uses of Cu@graphite core-shell nanostructures for enhancing optical nonlinearity and optical limiting capabilities.

O2- 0008

Plasmon-Enhanced Tunable Emission in MXene-Metal Nanoparticle Heterostructures

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Abstract

This study investigates the enhanced photoluminescence (PL) and redshift in emission wavelength resulting from the nanocomposite of MXene nanosheets with metal nanoparticles. MXenes, a class of 2D transition metal carbides, are known for their excellent electrical conductivity and optical properties. By integrating Nb2C MXene nanosheets with metal nanoparticles, we observed a significant enhancement in photoluminescence, attributed to the metal nanoparticles' localized surface plasmon resonance (LSPR) effect. The hybrid structures were synthesized through a sonication-assisted process, ensuring uniform dispersion of the nanoparticles on the MXene surface. Scanning electron microscopy (SEM) confirmed the successful decoration of MXene nanosheets with metal nanoparticles, revealing a uniform distribution across the surface. Photoluminescence (PL) spectroscopy showed a remarkable increase in emission intensity compared to pristine MXene, with a distinct redshift in the emission wavelength. This shift is likely due to the interaction between the excitonic states of MXene and the LSPR of the metal nanoparticles, resulting in energy transfer and recombination at lower energy levels. The synergistic effect of MXene's 2D structure and the plasmonic properties of metal nanoparticles pave the way for advanced optoelectronic applications, particularly in sensing, imaging, and light-emitting devices. The results demonstrate that MXene/metal nanoparticle heterostructure holds promise for engineering photonic devices with tunable optical properties.

O2- 0009

Influence of Szigeti effective charge on coherent Raman scattering In quantum plasma

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Abstract

By considering the quantum hydrodynamic model, an analytical study is performed to examine the impact of Szigeti's effective charge on coherent Raman scattering (CRS) of laser radiation in an unmagnetized direct band gap semiconductor. The CRS arising from electron density perturbations and molecular vibrations of the medium are produced at the transverse optical phonon frequency. The quantum hydrodynamic model of a homogeneous one-component (with electrons as carriers) system is considered to obtain the effective Raman susceptibility arising due to induced nonlinear current density and molecular vibrations. The effective charge of Szigeti plays a crucial role in determining the strength of the coherent Raman scattering signal, influencing the interaction between the laser radiation and the medium's vibrational modes. The Raman medium is a set of N harmonic oscillators with different frequencies and coupling constants. The equation of motion for a single oscillator (optical phonon) is given by [1].

$$\frac{\partial^2 u}{\partial t^2} - \omega_t^2 + 2\Gamma_a \frac{\partial u}{\partial t} = \frac{F}{M}$$

The quantum correction appears through the equation and includes two different quantum effects: (a) quantum diffraction and (b) quantum statistics [2].

$$\frac{\partial v_1}{\partial t} + \nu v_1 + \left(v_0 . \frac{\partial}{\partial x}\right) v_1 = \frac{e}{m} E_1 - \frac{1}{m n_0} \frac{\partial P}{\partial x} + \frac{\hbar^2}{4 m^2 n_0} \frac{\partial^3 n_1}{\partial x^3}$$

In this analysis, we obtained an expression for Raman gain coefficient (g_R) originating from the third-order susceptibility of the medium used in telecommunications that pumps lower-frequency photons to a higher-frequency regime. The dependence of (g_R) on wave vector, pump field strength and doping concentration in quantum plasma is reported for both cases viz., $(q_s = 0)$ and $(q_s \neq 0)$. Numerical estimations are made for a representative *n*-type InSb crystal duly shined by pulsed 10.6 μm CO2 laser.

O2- 0010

Photoinduced heat generation and transfer from single magnetite (Fe_3O_4) nanoparticles for optical hyperthermia applications

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Abstract

Plasmonic and magnetic nanoparticles generate heat through various mechanisms when illuminated, making them suitable for various biomedical and thermal applications. Among these, optical hyperthermia stands out for cancer treatment, enabling localized heating that selectively targets cancerous tissues. Iron tetroxide (Fe_3O_4) nanoparticles are gaining attention due to their magnetic properties and biocompatibility, which enhances their safety in biological environments and reduces the risk of adverse reactions. But the heat generation in Fe_3O_4 nanoparticles under optical illumination is not reported in the literature. This motivate us to do the theoretical study on heat generation and transfer in single Fe_3O_4 nanoparticles under UV to near-infrared light, comparing them with plasmonic (Au, Ag) and magnetic (Fe) nanoparticles.
We have systematically examined the optical absorption and scattering properties of nanoparticles of varying sizes. We analyze electric and magnetic field intensity enhancements both inside and outside the nanoparticles for different sizes and wavelengths. The influence of nanoparticle size and incident light wavelength on heat generation is assessed, followed by calculations of temperature increases in the surrounding medium. Notably, Fe_3O_4 nanoparticles demonstrate enhanced efficiency in heat generation and transfer when exposed to ultraviolet, visible, and near-infrared light, making them promising candidates for optical hyperthermia applications.

Keywords: Fe_3O_4 nanoparticles, Magnetic nanoparticles, Heat generation and transfer, Electric and magnetic field enhancement, Absorption, Scattering

O2- 0011

Observation and characterization of reflective whispering gallery modes of a photonic microresonator supported by a metal substrate: A theoretical study

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Abstract

Optical resonances or whispering gallery modes (WGMs) of single spherical-shaped dielectric microparticles have recently attracted researchers' attention due to their high-quality factor and low mode volume. In general, conventional WGMs (CWGMs) are formed due to the confinement of light by the total internal reflection of light at the periphery of the microparticles. The CWGMs are found useful in non-linear optics, fluorescence, Raman spectroscopy, photovoltaics, biosensing, electric field magnetic field sensing, pressure, humidity, temperature, and refractive index sensing etc.
It is to be noted that most of the CWGMs are confined inside the microparticles, and only the evanescent tail of the CWGM exists in the surrounding medium.This means that the electric and magnetic fields of the CWGM are not “fully accessible” for several applications. However, the evanescent field of the CWGM is much weaker than the internal field of the microparticles. Moreover, the evanescent decay length of the CWGM is too small. Due to these two reasons, the experimental signals are significantly limited because of restriction in the light-matter interaction. Therefore, herein, we report the generation and characterization of intense standing wave patterns or WGMs outside a single dielectric microsphere supported by a metal substrate for the first time. These WGMs can be called as “reflective WGMs (RWGMs).” The reflected light from the metal substrate plays an important role in the formation of the RWGMs. In contrast to the CWGMs, the electric and magnetic fields of RWGMs are “fully accessible,” and these can be utilized to enhance the light-matter interaction in several applications mentioned above.

O2- 0013

Aberration-free structured light in holographic optical tweezers

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Abstract

We present a method to generate aberration-free optical spots/structured light in a holographic optical tweezer system by optimizing a spatial light modulator (SLM) for global, spatial varying phase response (SVPR) and laser beam profiling across its spatial area. The correction for global and SVPR is incorporated through a modified weighted Gerchberg Saxton (WGS) algorithm to generate the optimized phase profile. Further, we present a technique to determine the incident laser intensity across the pixels of SLM used as an input to the WGS algorithm through the same diffraction setup. In general, the input laser beam profile to WGS or any structured light-generating algorithms is assumed centered to the SLM center, which may not match the actual incident laser beam centering. The effect of the mismatch of the actual laser beam center on SLM and laser beam center input to the algorithm is shown through the degradation of spot quality and uniformity in an array of eight focal spots in a circle. Further, having a technique to determine the laser intensity across the pixels of SLM allows the generation of aberration-free structured light with any transverse mode or an aberrated output of a laser in a holographic optical tweezer system.

O2- 0014

Soil Surface Parameter Monitoring via Microwave SAR Remote Sensing Techniques

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Abstract

The study of soil surface parameters is crucial for understanding various environmental processes, including soil moisture dynamics, erosion, and land-use changes. Microwave Synthetic Aperture Radar (SAR) remote sensing has emerged as a powerful tool for monitoring soil surface conditions due to its ability to penetrate cloud cover, operate day and night, and provide high-resolution data across large areas. This research focuses on the application of SAR remote sensing to evaluate key soil surface parameters such as soil moisture, surface roughness, and texture. By utilizing SAR data, particularly from sensors such as Sentinel-1, this study aims to develop methods for accurate and timely monitoring of these parameters across diverse landscapes.

The study emphasizes the advantages of microwave SAR in assessing soil properties, considering factors such as its sensitivity to dielectric properties and surface structure. Through advanced processing techniques, including backscatter analysis and polarimetric decomposition, the research explores the potential of SAR data in delivering consistent and reliable information on soil surface conditions. Case studies over varied terrains are conducted to validate the methodologies and assess the relationship between SAR-derived parameters and ground truth data. The results offer valuable insights for agricultural monitoring, hydrological modeling, and land management, demonstrating the importance of SAR remote sensing in soil surface studies.

O2- 0015

Remote Sensing-Based Compositional Mapping for Early Crop Disease Detection in VNIR Spectrum

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Abstract

Early detection of crop diseases is critical for ensuring agricultural productivity and reducing losses. This research focuses on compositional mapping of agricultural fields using spaceborne observations within the visible to near-infrared (VNIR) spectrum to detect early signs of plant stress and disease. Remote sensing techniques that utilize the VNIR spectrum can capture subtle changes in vegetation composition, which often precede visible disease symptoms. By analyzing multispectral and hyperspectral satellite data, this study aims to identify spectral signatures associated with crop diseases, enabling the development of early warning systems.

Advanced image processing methods, including vegetation indices such as the Normalized Difference Vegetation Index (NDVI) and Red Edge Normalized Difference Vegetation Index (RENDVI), are employed to detect anomalies in plant health. Spectral unmixing techniques and classification algorithms are used to map compositional changes at the field scale. The results provide actionable insights into crop health, facilitating early intervention and targeted disease management. This approach demonstrates the potential of spaceborne VNIR observations for real-time monitoring and precision agriculture applications, offering a scalable solution to improving crop disease detection and management.

O2- 0016

Dark-field microspectroscopic studies of single silicon nanoparticles fabricated by electron beam evaporation technique

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Abstract

Silicon nanoparticles (SiNPs) have attracted substantial attention and interest in the fields of nano-photonics, nanomedicine, and nanomaterials due to their exceptional optical properties and versatile array of applications such as photovoltaics, biosensors, bioimaging, drug delivery, and energy storage devices. The SiNPs are commonly observed in nanocluster films. These films can be deposited using plasma enhanced-chemical vapor deposition (PECVD), Hot wire CVD, gas-phase, microwave CVD, magnetron sputtering, laser ablation, and various physical vapor deposition (PVD) techniques. To optimize the performance of the SiNPs based devices, one should know the optical (absorption or scattering) properties of the SiNPs and the dependence of these properties upon the various experimental deposition parameters. To the best of our knowledge, the role of experimental parameters on the optical properties of single SiNPs is not reported.

Therefore, herein, for the first time, we report the effect of thermal annealing, deposition parameters, and polarization of light on the far-field optical properties of single SiNPs studied using a transmission-mode dark-field microscope. Initially, the SiNPs are fabricated using the electron beam evaporation technique using different deposition parameters, and their morphology is studied using an Atomic Force Microscope. Later, the scattering images and spectra of single SiNPs before and after the thermal annealing process are recorded using the dark field microscope. Finally, the polarization-dependent scattering images and spectra of single SiNPs are also recorded.

O2- 0017

Incorporation of Graphene Quantum Dots into Nematic Liquid Crystals for Improved Optical Limiting Application

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Abstract

Liquid crystals (LCs) are a unique class of materials that exhibit both fluid-like behavior and structured molecular arrangements, offering tunable optical properties through external stimuli. This study explores the linear and nonlinear optical behavior of a nematic LC (5CB) and its enhancement upon doping with graphene quantum dots (GQDs). Z-scan studies were conducted using 532 nm nanosecond excitation pulses to evaluate the nonlinear optical response. Our results demonstrate remarkable improvement in nonlinear absorption in the GQD-doped LC system, attributed to reverse saturable absorption. This effect arises from the interplay between excited-state absorption in the liquid crystal and two-photon absorption in the GQDs. Additionally, the interaction between the LC molecules and excited-state GQDs induces an anomalous reorientation of the LC molecules, further contributing to the observed nonlinear optical enhancement. We also report on the self-defocusing properties of both pristine and doped LCs, as analyzed through closed-aperture Z-scan measurements. The nonlinear tunability of the system was studied by applying varying voltages across the LC cell, revealing a dynamic control over the nonlinear optical responses. Such voltage-dependent behavior highlights the potential for these systems in advanced optical modulation applications.

O2- 0018

Study of 2D photonic crystal for optical devices using the base material of As_2Se3

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Abstract

In the present work, 2D photonic crystal structure is designed which consists of hexagonal lattice of air holes in As2Se3 matrix. In the structure, the waveguide is obtained by removing one row of air holes in X direction and, a microcavity is obtained at the centre of wave guide by removing two air holes in Z direction that produces a narrow peak in the transmission spectrum. The transmission spectra are obtained using finite difference time domain method (FDTD). The simulation results are studied by varying the size and position of the air holes in the matrix. The structure can be used in different optical devices.

O2- 0019

Review article for emission of single photon using carbon nanotube

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Abstract

Carbon nanotube had been used to produce single photon at room temperature. single photon emission based on atomic ensembles and spontaneous parametric down conversion, and then focus on solid-state emitters including semiconductor quantum dots, defects in silicon carbide and carbon nanotubes has been proposed [1]. The extensive characterization of carbon nanotube electron field emitters has been reported [2]. Comparative analysis of photoluminescence and upconversion emission from individual carbon nanotubes for bioimaging applications has also been proposed [3]. The major advancements in the field of SWNT (single-wall carbon nanotubes) biosensors over the last two decades with a focus given to recent advances in biological applications has also been reviewed [4]. The latest results in terms of single-photon purity, generation efficiency and indistinguishability has been described [5]. The Minireview discusses has been given into the electronic structure of carbon nanotubes obtained using single-molecule fluorescence spectroscopy [6]. By exploiting the cavity feeding effect on the phonon wings, the locking of the single-photon emission at the cavity frequency over a 4 THz-wide band while keeping the mode width below 80 GHz has also been proposed [7]. Enhancement for single-photon emission from carbon-nanotube dopant states coupled to silicon microcavities has been discussed [8]. Tuneable room temperature single photon emission at telcom wavelength from sp^3 defect in carbon nanotube at tunable room temperature has also been discussed.

O2-0020

Dual core Photonic Crystal Fiber Based Sensor for Detection of Fuel Adulteration with variation of concentration

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Abstract

In this paper, a dual-core photonic crystal fibre (DC-PCF) sensor is proposed featuring a rectangular analyte channel, designed for fuel Adulteration sensing. The cladding area of this sensor includes rectangular air holes. The proposed fiber uses silica as a substrate material, and it is operating within a wavelength range of 2 to 3 µm. PCF sensor has been analyzed by COMSOL Multiphysics software using finite element method (FEM). The obtained value of birefringence for x-polarised birefringence are 0.021191564, 0.021645186, 0.022581194, 0.023061401, 0.023872008, 0.024674917 and for y-polarised 0.0231, 0.023595313, 0.02458464**,** 0.02509149, 0.025950026, 0.026813163 for the different RI of petrol with concentration of kerosene at 0%, 20%, 40%, 60%, 80%, 100%. respectively**.** The values of coupling length for x-polarized are 70.78288425 µm, 69.29947249 µm, 66.42695744 µm, 65.04375016 µm, 62.83510042 µm**,** 60.79047766 µm and for y-polarized are 64.89583515 µm, 63.57194785 µm, 61.013707 µm, 59.78122386 µm, 57.80341007 µm, 55.942673129 µm at 0%,20%,40%,60%,100% concentration of kerosene respectively.The proposed PCF sensor tackles all the complexity faced by the ordinary sensor. The fabrication of this PCF sensor is not complex, and it can be built by the technique of 3D-printing, stakes building and many more. The high coupling length and low birefringence values helps to increase the sensitivity of the sensor and plays an important role in fuel Adulteration identification applications in future.

P1- 0001

Study of Structural, Optical and Shock Wave Influence of Oxalic Acid Crystals in Presence of Zinc Nitrate

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Abstract

In the present investigation oxalic acid crystals grown in presence of zinc nitrate were grown by slow evaporation solution method at room temperature. The crystallographic parameters of grown crystals have been determined by employing a single crystal X-ray diffraction study. The presences of a functional group were identified from FTIR vibrational spectroscopic technique. The optical transparency of the grown crystal has been examined in the range of 200-900 nm using UV-visible studies. The band gap energy is also calculated from the UV transmittance data and found to be 4.10 eV. The SHG efficiency of zinc nitrate oxalic acid crystal is 1.2 times higher than KDP. The subjected crystal also tested for PL and shock wave spectroscopic techniques. The thermal effect of zinc nitrate evaluated on dielectric traits of oxalic acid crystal has been evaluated by dielectric studies. The thermal behavior of BTNN doped KDP crystal has been analyzed by TGA/DTA analysis.

Keywords: Organic Single Crystal; Nonlinear Optics; UV-visible; PL; TGA/DTA.

P1- 0002

Analysis of Variation of Thermal Conductivity with Doping Concentration of High Temp Superconductor $La_{2-x}Sr_xCuO_4$

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Abstract

The theoretical analysis of heat transport in doped $La_{2-x}Sr_xCuO_4$ has been a source of discussion, particularly in superconducting region. The Quantum Dynamical approach has been put to test for calculation of thermal conductivity of $La_{2-x}Sr_xCuO_4$ for various concentrations of doping. The present study shows that the thermal conductivity of $La_{2-x}Sr_xCuO_4$ at x=0.01, 0.02, 0.04 and 0.1 can successfully explain the anisotropic behavior of these HTS. The conductivity decreases with increasing doping for single crystal which is in favor of other experimental findings. The present theory is applicable to all layered cuprate HTS. Further, the present study supports that the thermal conductivity along the CuO_2 layers is always greater than the perpendicular direction to the layers in the single crystal. At low temperature the phonon peak start disappearing with increase in doping concentration.

Q2- 0001

Controlling VO_2 Phase Stability by Cr Doping: An Insight Investigation by Advanced Synchrotron Spectroscopy

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Abstract

Being capable with strong electron correlation, Vanadium dioxide (VO_2) can undergo a volatile phase transition from the low-temperature monoclinic insulating phase to the high-temperature rutile metallic phase, occurring often simultaneously due to having insulator-to-metal phase transition temperature (T_{IMT}) at room temperature regime. The changes in the electronic structure associated with Cr-doping in epitaxial VO_2 thin films coherently deposited on *m*-Al_2O_3 (1-102) substrates by R-F Magnetron Sputtering. At 10 at% of Cr-doping, a metastable triclinic state is obtained due to phase transition from monoclinic (M1) state in pristine VO_2, while a first order monoclinic (*M2*) state is achieved after 30 at% of Cr-doping. The photo-emission spectra (PES) demonstrate the charge fluctuations observed in doped cases that produces Cr^{3+} and V^{5+} polarons that suppresses the insulating phase towards localization of the sites from $V^{4+} \rightarrow V^{4+}$ and $V^{5+} \rightarrow Cr^{3+}$ that is associated with Mott-Peierls' phenomenon suggesting the decrement of V-V dimerization with higher doping concentration. The X-ray absorption fine spectroscopic (XAFS) investigations combined with first-principles calculations, the atomic structural evolutions of Cr dopant and its role in tailoring the V-V dimerization can be unveiled. The characteristic spectral changes associated with Cr-doping and phase transitions cooperative with Mott-Peierls' IMT has been established by analyzing the local atomic structure and neighboring sites for individual elements via Near Edge and Extended-XAFS measurements. Our results show that the *M2* phase can be stabilized by chemical influence even at room temperature and possess identical electronic contributions other than *M1* and *T* and are also Mott-Hubbard insulators.

R1- 0002

Density Functional Theory and Molecular Docking Studies of Curcumin

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Abstract

Turmeric is a spice that has received much interest from both the medical/scientific world as well as from the culinary world and have medicinal properties known from thousands of year. Curcumin is the integral element found in it and is reported to have anti-inflammatory, antioxidant and anticancer properties. In the present paper we have studied three natural derivatives of turmeric namely Curcumin, Demethoxycurcumin and Bisdemethoxycurcumin. The structural properties have been studied by using Gaussian 09 and docking with protein 3NL1, X-ray crystal structure for Cox-2 Enzyme have been carried out by Autodock Vina.

The optimized molecular geometry has been used for molecular docking and for obtaining highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) which are important in predicting the chemical stability of the molecule. The energy gap between HOMO and LUMO is used to explain several chemical properties of a molecule namely; ionization Potential, Electron Affinity, Global Hardness, etc.

Molecular docking was used to study the possible interactions between Cox-2 protein (3LN1) and the selected curcumin derivatives. The binding sites were identified by using DoGSite tool of protein plus online server. The major purpose of the molecular docking analysis is to locate strong binding affinity (ΔG) and interactions between ligand and protein.

The result shows the binding energy of derivatives is almost same (≈ 9 kcal/mol). All the three derivatives show two common interactions with ARG106, HIS75. However Demethoxycurcumin shows higher number of interaction (6) with ARG106, HIS75, TYR341, GLH178, LEU338, SER339. Whereas Bisdemethoxycurcumin shows 5 and Curcumin shows 3 interactions with different Amino Acids. The results indicate that Demethoxycurcumin shows more potential to bind with target protein.

R1- 0003

Docking and Scoring of some Antitubulin Agents within taxol binding site incorporating a Model of Hydrophobic Enclosure

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Abstract

Cancer is a terrifying and heterogeneous illness characterized by uncontrolled cell growth which invades, erodes and destroys normal cells. Cancer treatment involves identifying and attacking cancer cells without harming normal cells. Now days, Taxol is a taxane chemotherapy drug. It's used to treat both early stage breast cancer and advanced, or metastatic, breast cancer. Taxol is a microtubule – stabilizing drug that stops cancer cell from dividing by binding to the microtubule agent. This prevents the chromosomes from segregating, which slow cell growth. A novel scoring function to estimate protein – antitubulin agent binding affinities has been developed and implemented as the XP scoring function and docking protocol. In order to this, Protein – ligand structural motifs leading to enhanced binding affinities are included Hydrophobic enclosure where group of ligand atoms are enclosed on opposite faces by tubulin protein atoms, neutral – neutral single or correlated hydrogen bonds in a hydrophobically enclosed environment, and five categories of charged-charged hydrogen bonds. The XP scoring function and docking protocol have been developed to reproduce experimental binding affinities for a set of 94 complexes and to yield quality enrichments for a set of fifteen screens of pharmaceutical importance. Enrichment results demonstrate the importance of the novel XP molecular recognition and water scoring in separating active and inactive ligands and avoiding false positives.

R1- 0004

Molecular Dynamic Simulation for Elastic Behaviour of $Cu_{1-x}Zr_x$

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Abstract

The $Cu_{1-x}Zr_x$ are formed using the molecular dynamic simulation in two different values of x. The formed alloys have been used to study the elastic behaviour of the alloys. The stress- strain diagram of the formed alloys has been plotted at four different temperatures. The effect of the temperature for each of the alloys have been compared. The effect of increase in proportion of Zr also presented in the study. Few of the Elastics constants/parameters also obtained for alloys under study. The Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) has been used for the present computation. The EAM potential for $CuZr$ alloys has been adopted as a force field exist in the alloys. The present article provides an effective comparative study of the Cu- based alloys at different temperatures for different proportion.

R1- 0005

Nanoscale Wettability of Water-Alcohol Mixtures on Graphite Surface: Molecular Dynamics Study

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Abstract

The ability to predict and control surface wettability at the nanoscale is crucial and rapidly evolving, particularly in the fields of microfluidics and nanotechnology. Typically, the contact angle is measured in simulations by creating a liquid droplet on a solid surface, fitting a curve to the droplet's interface, and determining the angle at the triple-phase contact line. However, at the molecular level, the triple-phase contact line becomes ambiguous due to the continuous motion of molecules, making conventional measurements difficult. This study reports the molecular dynamics simulations to determine the contact angle of water mixed with four primary alcohols (R_N-OH, where R = (C_NH_{2N+1}), N varies from 1 to 4) on a graphite substrate, using the Hautman and Klein method, which links the microscopic contact angle to the droplet's average center of mass height through the concepts of equivalent contact area and volume. The water concentration is varied from 50% to 90% in the alcohol mixture. ContactAngleCalculator code is modified to calculate the contact angle of binary liquids. Results show that increasing alcohol concentration leads to greater spreading.

R1- 0006

Fe2-xCoxHfSi Heusler alloys as potential candidates for MTJ layers: a DFT study

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Abstract

Magnetic tunnel junction (MTJ) devices which exhibit much larger magnetoresistance as compared to the GMR based devices offer significant possibilities in spintronics as magnetic storage device, magnetic read-heads, spin injectors and spin filters. For these devices to work as a spin-switch, a semiconductor layer is sandwiched between two half-metallic layers providing a flow of pure spin current. Fe2-xCoxHfSi full Heusler alloy series has been investigated as potential candidate as all Heusler MTJ device. Density functional theory-based calculations with full potential linearized augmented plane wave approach reveals both semiconducting and halfmetallic members from the studied series of alloys possessing large values of half-metallic bandgap and lattice mismatch of only 1%. The electronic and magnetic properties show the existence of magnetism due to the exchange splitting of the 3d-eg orbitals of Co and Fe atoms. The magnetic moment in different doped alloys varies as a function of valence electron count. The robustness of the half-metallicity of Co2HfSi is confirmed for a large variation of lattice parameter (-8% to +11%). Several 48 atom MTJ cells were formed with the base configuration of Co2HfSi-Fe2HfSi-Co2HfSi. Different interfacial defects such as single and double atomic swapping were also investigated for a detailed analysis which provided sufficient evidence to support these full Heusler series as potential MTJ layers.

R1- 0007

Role of projectile ion mass in vacancy formation on muscovite mica

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Abstract

Muscovite mica [$KAl_2(Si_3Al)O_{10}(OH)_2$] is a layered, multi-elemental, electrically insulating material with an atomically flat surface. Due to such unique properties, mica is applicable for different applications. The introduction of defects can tailor the properties of mica drastically. This study explores the impact of projectile ion mass on defect and vacancy formation in muscovite mica using Monte Carlo simulation. Low-energy irradiation (10 keV) with Ar^+ and O^+ ions at normal and near-grazing incidence is considered. Results show varying vacancy formation in mica's constituent elements, with heavier Ar-ions inducing maximum vacancy production. Despite similar total energy transfer, damage, and vacancy production differ across ions. A shift in the ion distribution profile towards deeper penetration depths is observed. SRIM simulations based on the NRT displacement model provide a qualitative explanation for vacancy formation, considering the energetic ion's energy transfer. The study sheds light on the interplay between projectile mass, energy transfer, and vacancy formation in muscovite mica. Ar^+ ions, being heavier, exhibit greater damage due to higher transferred energy, leading to increased vacancy formation. The displacement energy for oxygen atoms is larger, resulting in higher oxygen vacancy in muscovite mica compared to other elements. The available energy for creating damage (T_{dam}) is greater for Ar^+ ion bombardment compared to other ions. This leads to more vacancy formation compared to other ions.

R1- 0008

Flow Behaviour of Harmful Gases Emitting From Mineral Ore Mines

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Abstract

The prime safety of the mine workers and the engineers working in the underground mines of various mineral ores is a matter of concern. This work emphasizes on the releases of different pollutants and their impact on the health of mines. Also, the researcher investigates the flow dynamics of the pollutants emitting from the mineral ore mines. The hazardous gases and particulate matter poses a random character as such the mining process requires the application of both modern ventilation system and safe methods in order to minimize and safeguard the health of workers working in the mines. Following features are covered in this research work such as advanced ventilation system and their deign with working efficiency parameters in underground as well as open – pit mines. Also different computational fluid dynamics mine ventilation and methodology for mine ventilation with different plume behaviors are summarized in this research work. Finally. Recommendations for the installation of future AI (Artificial Intelligence) based ventilation system and health safety devices of workers are given in the concluding remarks.

Keywords: Pollutants, mineral ore, hazardous, ventilation, open – pit , Artificial Intelligence

R1- 0009

Investigating the salt dependency of glass transition temperature in EC-LiTFSI electrolytes

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Abstract

Concentrated electrolytes hold significant promise for enhancing battery stability and performance, with the glass transition temperature (Tg) serving as a critical factor influencing both mechanical stability and ionic conductivity. In this study, we investigate the dependence of Tg on salt concentration in EC-LiTFSI electrolytes, utilizing molecular dynamics simulations across concentrations ranging from 0.005 M to 2.5 M. Our results indicate that the Tg for a 1 M ECLiTFSI solution is 229 K, consistent with previous simulations but slightly higher than experimental predictions, highlighting the need for further investigation into the underlying mechanisms. We predict that Tg increases with salt concentration, saturating beyond c = 1.4 M, as described by the equation: $T'' = T''\$ + \Delta T'1 - e+,/,./$, where $T''\$$ = 183.8 K, ΔT = 80.8 K, and $c\$$ = 1.4 M. This study reveals a monotonic increase in Tg with salt concentration, providing valuable insights into optimizing the ionic conductivity and mechanical properties of EC-LiTFSI electrolytes. Understanding the interplay between Tg and the diffusion coefficient is crucial for enhancing the performance of these electrolyte systems in practical battery applications. Fig.: Glass transition temperature (Tg) of EC-LiTFSI electrolytes as a function of salt concentration. Circles represent simulation data, while the solid line corresponds to the fitted equation: $T'' = T''\ \$ + \Delta T'1 - e+:/:./$, c is the salt concentration.

R1- 0010

Salt concentration effects on the glass transition temperature of PEO-NaPF6 electrolytes: insights from molecular dynamics

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Abstract

Sodium-ion polymer electrolytes have gained attention as a cost-effective and environmentally friendly alternative to lithium-ion batteries, offering enhanced safety, mechanical stability, and biodegradability. A key parameter influencing the performance of these solid-state electrolytes is the glass transition temperature (Tg), as it impacts both mechanical stability and ionic conductivity. In this study, we performed atomistic molecular dynamics simulations to investigate the Tg of PEO-NaPF6 electrolytes and its dependence on salt concentration. At an EO:Na ratio of 15:1, the Tg was found to be 287 K, higher than that of neat PEO due to strong polymer-ion interactions that restrict polymer chain mobility. Our simulations show a monotonically increasing trend in Tg with increasing salt concentration, which saturates beyond a critical point, fitting the relation $T'' = T'' \$ + \Delta T'1 - e+,/,./$. Furthermore, we explored the relationship between Tg and ion diffusion, finding significant positive correlations, which are crucial for optimizing the mechanical and ion-conducting properties of PEO-NaPF6 electrolytes. These findings contribute to a deeper understanding of how tuning Tg and diffusion coefficient can enhance electrolyte performance in sodium-ion batteries.

R1- 0011

Computational Algorithms for Biospeckle Signal Analysis & Evaluation: Review

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Abstract

The biospeckle technique is a non-destructive and optical technique used for the analysis of the activity of biological samples based on the pattern received on screen via a backscattered laser beam from the sample. This technique has been successfully applied in various domains like medicine, agriculture, and microbiology. In this paper, we perform a survey focused on the computational models and algorithms used for the analysis of speckle signals. We examine the biospeckle acquisition process, specific methods, models, and simulations. This paper explored the biospeckle signals analysis using machine & deep learning-based computational models. Moreover, we presented some application areas where machine and deep learning-based computational models deployed for the classification and analysis. Our findings indicate that machine and deep learning-based models provide automated classification and analysis of biological processes using biospeckle signals and images, outperforming existing commonly used signal/image processing techniques

Keywords: Biospeckle, computational models, biological processes.

R1-0012

Spectroscopic, Thermodynamic properties and Fukui Function analysis of pentahydroxyflavane

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Abstract

In the present work, the compound pentahydroxyflavane is studied experimentally and theoretically. The calculations have been performed to compute optimized geometry, atomic charges and thermodynamic properties using Hartree Fock Theory (HF) and Density Functional Theory (DFT) with 6-311G basis set. The redistribution of the electron density (ED) in various bonding and antibonding orbitals and E(2) energies have been calculated by natural bond orbital (NBO) analysis to give the clear evidence of stabilization originating from hyperconjugation of various intra- molecular interactions. The calculated HOMO-LUMO energies show that the charge transfer occurs within the molecule. The HOMO-LUMO energies, the temperature dependence of the thermodynamic properties and the Fukui functions of the title compound are also studied. The vibrational analysis of the compound has also been carried out.

Keywords: FTIR, VEDA, NBO, HOMO-LUMO, Fukui Function.

R1-0013

Buckling Analysis of Porous FGM Plate using First Order Shear Deformation Theory

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Abstract

The buckling analysis of porous rectangular FGM plate is presented. The finite element method based on first-order shear deformation plate theory is used. The FGM plate with even type porosity is modeled as a laminate with perfectly bonded isotropic layers. The material properties at middle of each layer are calculated using power law and rule of mixture. After validating the present formulation with previous literature various parametric studies are conducted to revel the effect of various parameters, viz. material gradation exponent, geometric variables, and porosity, on the buckling response of the FGM plate. It is found that the material gradation exponent has a noticeable effect on the buckling strength of FGM plate. Further, with the increase in the porosity leads to monotonic decrement in buckling strength of FGM plate. It is also shown that the aspect ratio of rectangular FGM plate considerably affects the buckling behavior of FGM plate.

Keywords: Functionally graded material (FGM), Buckling behavior, Porous FGM plate, Finite element analysis, FSDT(First Order Shear Deformation Theory).

R1- 0014

Predicting band gaps of Janus MXenes: an account from machine learning and first-principle DFT studies

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Abstract

This work is primarily focused on predicting the band gaps of Janus MXenes from machine learning (ML) models. Five supervised ML models such as multi-layer perceptron (MLP), gradient boosted decision tree (GBDT), random forest regression (RFR), extreme gradient boosting (XGBOOST) and gaussian process regressor (GPR) have been considered to predict the band gaps of the said systems. The accuracy of each model has been tested from mean absolute error, root-mean-square error and determination coefficient R_2 values. Among all the five ML models XGBOOST algorithm shows highest R_2 value (=0.95). Additionally, structural, mechanical properties and electronic band structures of the Janus MXenes have been studied in detail from density functional theory (DFT) calculations. The band gap values of the compounds have been estimated from DFT calculations at HSE06 level of theory. The present study will be helpful in exploring the ML models in predicting the band gaps of Janus MXenes which in turn may bear potential applications in optoelectronic, piezoelectric devices.

R1- 0015

Forecasting the Antimicrobial Activity of Silver Nanoparticles by utilizing Machine Learning

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Abstract

Silver nanoparticles are widely recognized for their ability to combat bacteria and fungi, making them promising candidate for antimicrobial research. Incorporating machine learning learning methods for the prediction of antimicrobial studies helps in increasing the medical applications of silver nanoparticles by offering a more efficient and cost-effective substitute to conventional laboratory experiments and finds diverse advantages especially in the cost reduction in the production of antimicrobials and minimization of trial and error of the traditional laboratory experiments. In this work, we introduced machine learning for the prediction of antimicrobial properties of silver nanoparticles. The datapoints for the machine learning modelling were collected from literature review. In the study, a range of machine learning regression models were employed to pinpoint the most effective one for predicting antimicrobial activity with greater accuracy. The machine learning models employed for the study includes Random Forest, AdaBoost and XGBoost machine learning algorithms. The efficiency of these machine learning models was confirmed through performance metrics. Since we do the random split of data into training and test sets, we can have multiple realisations of test and train data sets with having the same split ratio of 0.1. As such, we have simulated over 10 realisations of each model. Utilizing these metrics, the models that provided the best predictions for antimicrobial activity were determined. And we got the XGBoost model with 0.93 coefficient of determination. The result of the simulation is depicted in the table below.

R1- 0016

Analysis of Functionally Graded Turbine Blades under Themo-Mechanical Loading Conditions Using Finite Element Method

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Abstract

This paper presents a comprehensive thermo-mechanical analysis of turbine blades composed of Functionally Graded Materials (FGMs) under thermal loading conditions using the Finite Element Method (FEM). The analysis employs a two-noded shear-deformable beam element with material properties graded continuously through the thickness of the FGM blade. The spatial variation of material properties is modeled using a Power Law distribution, and the Voigt model is applied to accurately predict the effective Young's modulus and thermal expansion coefficient across the FGM structure. The accuracy of the developed finite element formulation is validated through a comparative analysis with benchmark solutions from existing literature. An extensive parametric study is conducted to evaluate the influence of varying material gradients, geometric configurations, and thermal loads on the stress distribution and deformation behavior of the turbine blade. The results, presented in both graphical and tabulated forms, demonstrate that the use of FGMs significantly enhances the thermal resistance and mechanical performance of turbine blades, thereby highlighting their potential in improving operational durability under extreme working conditions.

Keywords: Thermo-Mechanical Analysis, Functionally Graded Materials, Finite Element Method, Turbine Blades, Power Law and Voigt Model.

S1- 0001

First and Second Order Topological Phases on Ferromagnetic Breathing Kagome Lattice

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Abstract

In this work, topological properties of a ferromagnetic Heisenberg model on a breathing kagome lattice are investigated extensively in the presence of Dzyaloshinskii–Moriya interaction. While the kagome ferromagnet hosts only a single first order topological phase, the breathing kagome system exhibits multiple first and second order topological phases along with their coexistence. Magnon dispersion relation is obtained by using linear spin wave theory. Flat band and Dirac cones are obtained in the absence of Dzyaloshinskii Moriya interaction. A topological phase diagram is presented where several first and second order phases as well as their overlap are identified. Values of thermal Hall conductivity for all the first order phases are obtained. Distinct first order phases are characterized by different sets of Chern numbers in association with the necessary chiral edge states in accordance to the first order bulk-boundary-correspondence rule. Second order phase is characterized by polarization along with the emergence of corner states. Violation of the second order bulk-corner-correspondence rule has been noted in some regions.

S1- 0002

Understanding defects states passivation in WSe_2 monolayer using Oxygen doping

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Abstract

Defects engineering is a well-established strategy to tailor the electronic structure and optical properties of materials. In two-dimensional (2D) semiconductors such as MoS_2, WSe_2, WS_2, $MoSe_2$ etc., defects are prevalent, therefore achieving precise control over defect formation and passivation remains a notable challenge. Here, in this work, we investigated various intrinsic defects states such as Sulphur vacancies (V_{Se}), tungsten vacancies (V_W), antisite defects (W_{Se}, Se_W) in WSe_2 monolayer using Density Functional theory (DFT) calculations. It is well known that the 2D materials are prone to unintentional chemical interactions with molecular oxygen (O_2) being a common source of contamination in ambient conditions. Therefore, we have simulated defected WSe_2 monolayer with Oxygen (O) doping where one Se atom replaced with O atom i.e. O_{Se}. The formation energy of O_{Se} in W-rich and Se-rich is calculated and it is observed that the formation of O_{Se} is exothermic in nature. From the electronic band structure of O_{Se}-doped WSe_2 monolayer, no gap states are observed which indicates that incorporation of oxygen can be used to passivate V_{Se} in monolayer WSe_2.

S1- 0003

Structural and Electronic Properties of Zigzag Gallium Nitride Nanoribbons Functionalized with Br

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Abstract

Nanoribbons, the quasi-one-dimensional structures present entirely novel properties as compared to their two-dimensional (2-D) counter parts due to unique electron confinement. Furthermore, the presence of edges provides an easy way to tailor their electronic properties via chemical edge functionalization. In this direction, we have systematically investigated the effect of Br-edge functionalization on the structural and electronic properties of zigzag GaN nanoribbons (ZGaNNR). Present analysis were performed with first-principles calculations using density functional theory (DFT) and the findings were compared with bare and hydrogen functionalized ZGaNNR structures. To comment on the dimensionality effects, nanoribbons having widths Nz = 4, 6, 8 were considered. It is revealed that Br functionalization is mediated via stable chemical bond formation with the edge atoms of the ribbons. Our Stability analysis shows the Br functionalization significantly improves the structural stability even more than that of widely reported H functionalization. However, a small distortion is witnessed in the optimized geometries of Br-functionalized ZGaNNR. H-functionalized ZGaNNR are well known wide band gap semiconductor, however, Br-functionalization leads to significant reduction in the band gap. The obtained band gaps in Br-functionalized ribbons lie between 0.74 eV to 0.19 eV. Overall, our study predicts that Br functionalization of ZGaNNR would be fruitful for the band gap engineering of ZGaNNR for various technological applications.

Keywords: GaN, nanoribbon, electronic structure, density of states, functionalization.

S1- 0004

Charge transport mechanism of low ion beam implanted chemically reduced graphene oxide by variable range hopping model

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Abstract

The Chemically assisted graphene oxide is synthesized by Improved Hummers' method and reduced by hydrazine hydrate to form reduced graphene oxide. The chemically reduced graphene oxide is further reduced by low energy (50 keV) Nitrogen (N+) ions beam implantation for better conductivity. The Raman spectra of all the samples consist of D-band and G-band at 1360 and 1590 cm-1 respectively which keeps on merging with implantation doses. The merging of D and G bands with high implanted doses reveal the surface amorphization effect. It is explained on the basis of shifting of G band towards lower frequencies and the D band towards higher frequencies. The reduction of all the samples has been estimated by the Tuinstra and Koenig relation to calculate the relative size of the sp2 carbon domain. The room temperature dc conductivities of reduced graphene oxide samples are found to be increases with reduction from 2.5 x 10-2 to1.94 S/cm. The dc conductivity of reduced graphene oxide has been reported in the temperature range of 77 to 400K on the basis of 3D variable range hopping (VRH) model.

S1- 0005

Morphological evolution of MoSe2 flakes synthesized by NaCl-assisted chemical vapour deposition

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Abstract

MoSe2 is a typical two-dimensional (2D) transition metal dichalcogenide (TMDC), which has garnered significant interest in recent years due to its semiconducting properties and tunable band gap with potential applications in optoelectronics, photocatalysis and atomically thin devices. In this study, we report the controlled synthesis of MoSe2 films using an indigenous atmospheric chemical vapor deposition (APCVD) system. NaCl is employed as a seed promoter to facilitate the growth of large-scale monolayer, bilayer, and multilayer films. The addition of NaCl leads to the increased surface mobility of precursors and can enhance the lateral growth of the as-grown domains. We present systematic studies to control the shape evolution of MoSe2 nanostructures by tuning different growth parameters. High-resolution optical microscope images reveal diverse MoSe2 morphological features, which include nanoribbons, snowflakes, web-like structures, monolayers and multilayer polygonal domains. A growth mechanism is proposed to understand the formation of these nanostructures. Additionally, field emission scanning electron microscopy (FESEM), Raman spectroscopy, X-ray photoelectron spectroscopy (XPS) and Atomic Force Microscopy (AFM) were employed to characterize the as-grown MoSe2 films. Our findings highlight the prospects for the controlled growth of novel 1D and 2D TMDC nanostructures and could enrich the understanding of the growth of TMDCs for a variety of device applications.

Keywords: MoSe2, Chemical vapor deposition, NaCl, nanoribbons, snowflakes.

S1- 0006

Ultrafast Electrochemical detection and determination of Uric Acid through modified 2D material based Pencil Graphite Electrode

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Abstract

Uric Acid (UA) is a very common antioxidant and a natural waste product obtained from metabolic breakdown and its appropriate levels in blood and urine samples are predefined. High blood plasma levels of UA contribute to hyperuricemia, which raises the risk of cardiovascular illness, Lesch-Nyhan syndrome, type 2 diabetes, and gout. Conversely, Parkinson's, Alzheimer's, and multiple sclerosis have been linked to low levels of UA. Conventional methods had limitation of cost and time. However, technological development and available fast detection electrochemical method mainly, Cyclic voltammetry (CV), is one of the easier and swift methods to detect and determine target material with a good amount of sensitivity. A facile electrochemical approach has been used in this study to detect and determine uric acid in biological samples and food products through Nitrogen and Sulfur co-doped reduced graphene oxide (NS-G) modified eco-friendly pencil graphite electrode (PGE). The morphological and crystallographic structure of NS-G has been confirmed using scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), Raman spectroscopy and X-ray diffraction (XRD). A comparative study of NS-G modified PGE's with N-G modified PGE's has also been carried out. The results show consistent stable voltammetry measurement confirming a reliable performance with lower limits of detection.

S1- 0007

Reduced graphene oxide/MnO_2 composite films as the electrodes for high-performance supercapacitors produced by successive ionic adsorption and reaction (SILAR) method

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Abstract

In the present work, the successive ionic adsorption and reaction (SILAR) method has been used to prepare rGO/MnO_2 (SL-GMN X) composites films on stainless steel (SS) substrate for three different number of cycles (X= 10, 15, and 20). This synthesis method provides a binder-free route. The composition and structure of MnO_2 and SL-GMN X composites films were characterized by X-ray diffraction (XRD), Fourier transforms infrared spectroscopy (FTIR), energy dispersive X-ray analysis (EDAX), and X-ray photoelectron spectroscopy (XPS). The morphology of samples is analyzed by transmission electron microscopy (TEM) and scanning electron microscopy (SEM). Surface area and porosity measuments are analyse using Brunauer-Emmett-Teller analysis (BET). The high surface area and abundant porosity of SL-GMN 15 enable more adsorption sites to shorten the ion diffusion pathway. Electrochemical studies investigated that SL-GMN 15 composite film displays excellent specific capacitance of 424 Fg^{-1} in three electrodes configuration with 1M Na_2SO_4 aqueous electrolyte. SL-GMN 15 composite symmetric supercapacitor displays a high specific capacitance of 117 Fg^{-1} and possesses maximum energy density with 16.3 $Whkg^{-1}$ at a charging current of 1 mA. Furthermore, the composite exhibits long cycle life and 99.5% specific capacitance maintained after 5000 cycle tests at a charging current of 3 mA. These results open the way for development of rGO/MnO_2 composite electrodes for supercapacitors and other energy storage applications.

S1- 0008

Electronic and Mechanical Properties of Janus Si_2OS Monolayer: A Promising Piezoelectric Material for Nanodevices

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Abstract

A class of materials known as 2D Janus monolayers exhibit a number of properties due to the breakdown of inversion and mirror symmetry. This class of materials can easily exhibit out-of-plane piezoelectricity. In this study, we examined the electronic structure, mechanical properties, and piezoelectricity of the Janus Si_2OS monolayer using first principle with Quantum Espresso. We optimized the cell parameters using different pseudopotentials in order to align our results with previous studies. Our electronic calculations with pbsol-Projector-Augmented Wave (PAW) pseudopotential indicate an indirect band gap of 1.31 eV. Elastic constants calculated in this study are in agreement with previous studies. In our investigation, we found that the Si_2OS Janus monolayer demonstrates piezoelectricity under stress, suggesting it is a potential candidate as a lightweight, high-performing piezoelectric nanodevice material.

S1- 0009

Electronic and Mechanical Properties of Puckered GeTe and $GeSnTe_2$ Monolayers

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Abstract

In recent years, it has become increasingly evident that two-dimensional nanomaterials have inherent piezoelectric properties, which have now attracted significant interest for their potential applications in next generation piezoelectric devices. The puckered structure of GeTe monolayer that demonstrates gigantic piezoelectricity motivated us to compare the properties of GeTe and $GeSnTe_2$ monolayers. In this study, we studied the puckered structure of both the monolayers, through Quantum Espresso; we investigated their electronic properties, such as the band structure and density of states. Our calculations show a very small effect on the band-gap on adding Sn atoms to GeTe monolayers, which was 0.92 eV for GeTe and 0.90 eV for $GeSnTe_2$, and this aligns with the previously reported work. The elastic constants of the two monolayers were then compared, and it was found that Young's modulus varies very little but shear modulus and Poisson ratio were drastically different in $GeSnTe_2$. The effect of strain on the band gap and effective mass has been studied and then we compared the piezoelectric coefficients of both the materials.

S1- 0010

Bandgap engineering in two- dimensional dichalcogenide semiconducting alloy

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Abstract

Alloying in two-dimensional transition metal dichalcogenides (TMDs) for eg. $MoSe_2$ and MoS_2 can occur in various ratios of sulfur and selenium, allowing for tunable electronic and optical properties. Due to its tunable properties, Molybdenum sulphur selenide (MoSSe) has been explored for applications in transistors, photodetectors, and catalysts. Monolayer and few layers $MoSe_2$ has been synthesized on cleaned 300 nm SiO_2/Si substrate by Chemical Vapor Deposition (CVD) method using a two-zone horizontal tube furnace with 50 mm diameter quartz tube. Raman spectrum is found to be highly composition concentration dependent. Two vibrational modes, $A_{1g\ (Se\text{-}Mo)}$ and $E_{1g\ (Se\text{-}Mo)}$ were observed at lower frequencies. This is consistent with the fact that with increase in Selenium content, the interaction between Sulfur and Selenium would softens the S-Mo related modes and at the same time, Se-Mo related modes are reinforced until the binary $MoSe_2$ is formed. Monolayer $MoSe_2$ shows a prominent peak at 802 nm in photoluminescence spectroscopy. This peak is red shifted for MoSSe. A highly intense emission peak at 762 nm (1.62 eV) is observed for as-grown composition modulated alloy.

T1- 0001

Effect of wire arc additive manufacturing on microstructure and mechanical properties of Duplex Stainless Steel – A Review

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Abstract

Metal additive manufacturing (AM) provides remarkable design flexibility; however, the high thermal gradients involved can lead to non-equilibrium microstructures characterized by chemical and interfacial instabilities. In the case of steels, this can result in unique microstructural features and potential performance challenges. The present investigates the impact of Wire Arc Additive Manufacturing (WAAM) on the microstructure and mechanical properties of Duplex Stainless Steel (DSS) 2205. The research highlights the advantages and challenges of WAAM in producing SS 2205 components, with a focus on microstructural evolution, phase distribution, and resultant mechanical characteristics such as Hardness, Tensile strength and percentage of elongation.

T1-0002

Review of rail wheel manufacturing process (Forging & Casting)

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Abstract

The manufacturing of railway wheels is essential to the functioning of the global railway industry as they are a vital part of the transportation infrastructure. This paper gives a detailed analysis of the two major manufacturing techniques applied in the railway wheel industry: forging and casting. Forging involves heating ingots and then mechanically deforming them while hot to produce high-strength wheels for heavy loads, high-performance environments, and impact resistance. Casting involves pouring molten metal into molds to produce complex geometries of the wheel, which have flexibility in design but less strength overall than forged wheels. Depending upon the application, materials used in these processes include carbon steel, alloy steel, cast iron, high speed steel, etc. Forging produces rail wheels with excellent strength and resistance to wear and fatigue, making them ideal for high speed and freight applications. Castings are less durable but offer cost-effective production for low stress applications. The paper also mentions the mechanical properties, chemical composition, and heat treatment methods applied to each process besides a quite detailed analysis regarding associated forging defects and how to avoid them. The study ends by comparing the advantages and disadvantages of the two production methods offering an idea concerning the way flow and the skin affect the final results of the railway wheels.
This paper lists some of the achievements in rail wheel production, most importantly being its process optimization through final elemental analysis, innovative design, and an integration of automatic learning methods. These technological developments have improved the safety, efficiency, and reliability of modern rail wheels as compared with all the severally high demands of contemporary rail transport systems.

Keywords: Rail Wheel, Forging, Casting, Carbon Steel, Mechanical Properties.

T2- 0001

Antimicrobial Efficacy of Low-Pressure Argon Plasma on Mobilized and Immobilized E.coli

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Abstract

This study investigates the antimicrobial efficacy of low-pressure argon plasma on *Escherichia coli* (*E. coli*) immobilized on glass substrates as well as mobilized in LB media. The bacterial cultures were exposed to argon plasma at 100 mW with a 50 sccm gas flow for 1 to 5 minutes. Optical Density (OD) measurements at 600 nm were taken throughout the bacterial growth curve and post-plasma treatment, while Atomic Force Microscopy (AFM) was employed to evaluate morphological changes in bacterial membranes across various scales (20×20 µm, 10×10 µm, 5×5 µm, and 2×2 µm). AFM scans revealed increasing membrane roughness with longer plasma exposure, particularly evident in the smallest scan sizes where height fluctuations were demonstrated. Optical Density (OD) measurements after plasma exposure demonstrated a significant reduction in bacterial viability, with the normalized OD decreasing progressively from 1.00 to 0.57. These results suggest that low-pressure argon plasma effectively disrupts bacterial membranes in solid film, leading to a marked decrease in cell viability with suspended form in liquid. The findings emphasize the potential of low-pressure argon plasma as an effective antimicrobial method for surface sterilization.

T2- 0002

Radiation Therapy Set-Up Error Study & its Impact on Treatment Delivery Accuracy

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Abstract

In radiotherapy, set-up errors are frequently found in several forms in the radiation treatment delivery process [1]. Delivering the appropriate amount of radiation to the target cells by protecting vulnerable organs is the critical goal of radiotherapy. Due to technological advancement, image-guided radiotherapy (IGRT) could achieve a far better accuracy for set-up as well as delivery [1]. Still, the external body mismatch between the planned computed tomography (CT) image and the XVI cone beam computed tomography (CBCT) image can be caused by a number of variables, including body weight loss and mechanical or physical set-up errors [2]. Since there is variation in the voxel matrix patient model, a discretized patient representation, this can alter the actual dosage calculation and its dosimetric impact on the illness site and other organs at risk. Additionally, the patient's body exhibits non-homogeneity and abnormalities in several sites, including the chest, abdomen, and lungs [2]. This discrepancy could lead to a greater inaccuracy in the dosage that the doctors recommend. The purpose of this study is to determine how much the patient's body changed in dose distribution and how much the dose varied. The Gamma Analysis pass-fail criterion for patient-specific Intensity Modulated Radiotherapy (IMRT) quality assurance (QA) is being used in this study [3, 4] and we found that the gamma passing rate gets reduced depending on the variation in the patient's body. The study would find out the quantitative evaluation of dose distribution variations [3, 4] due to a mismatch in the patient's body or external between the planning CT image and XVI (CBCT) image acquired before treatment. This research will help identify the best ways to prevent these setup mistakes so that patients can receive more precise therapy going forward.

Keywords: Computed tomography, Cone beam computed tomography, Intensity Modulated Radiotherapy, Image-guided Radiotherapy

T2- 0003

Anti-Fungal Activity of Different Phytochemicals against *Malassezia sp.*

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Abstract

A frequent ailment that affects the state of the scalp is dandruff. Dandruff can only be adequately managed; it cannot be entirely eradicated. Products that are currently on the market perform poorly or cause symptoms to return. Plant extracts contain a variety of active substances that might aid in preventing the establishment of resistance in the causing organism. Therefore, the goal of the current study is to develop a poly-herbal blend that may be added to hair oil to improve its anti-dandruff effectiveness. This mixture will be rich in alkaloids, flavonoids, phenolic compounds, terpenoids, and tannins. Therefore, the present study deals with the computational analysis of the interaction of the phytochemicals present within margosa, rosemary, chamomile and tea tree against *Malassezia globosa*.

T2- 0004

Assessment of normal tissue objective function using intensity modulated radiosurgery of single brain metastasis

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Abstract

Efficacy of radiosurgery planning in terms of normal tissue sparing and tumor dose conformation is essential for favourable treatment outcomes. This study examined normal tissue objective function (NTO) by assessing its variations for radiosurgery planning of single brain metastasis with intensity-modulated and volumetric-modulated arc radiosurgery techniques. The NTO function is an exponential function based on of dose and distance parameters such as start-dose (Ds), end-dose (De), start-distance (x_i), slope (k) and priority. Twenty cases were retrospectively planned with IMRT and VMAT techniques. The applied NTO parameters were Ds = 99%, De = 10%, x_i = 1 mm k = 1.0 mm^{-1}, and priority = 100. All targets were planned using 20 Gy margin dose while maximum dose was constrained to 25 Gy. The resulting plan types were analysed using normal brain receiving 12 Gy (V12), gradient index (PGI), conformity index (PCI), prescription isodose level (PIDL), and MU/Gy. Normal brain dose was significantly lower for VMAT plans compared to IMRT plans. V12 was lower by 1.5 cm^3 for the VMAT plans, $P < 0.001$. PGI was better for VMAT (2.9 ± 0.3) than for IMRT (3.5 ± 1) for all planned cases, $P = 0.0025$. PCI was comparable between IMRT and VMAT plan types. Mean PIDL was also similar, at about 70%, for both techniques. MU/Gy was significantly lower for IMRT compared to VMAT, $P < 0.001$. The NTO based modulated radiosurgery techniques exhibited varied dosimetry. VMAT plans showed overall betterment in dosimetry compared to IMRT plans.

T2- 0005

Docking Study of Natural Products as Potential Antitubercular Agents

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Abstract

Tuberculosis (TB), caused by *Mycobacterium tuberculosis*, continues to be a major global health concern, exacerbated by the rise of drug-resistant strains and the limitations of existing treatments. Natural products have historically been a valuable source of therapeutic compounds. This study investigates the potential of various natural products as antitubercular agents through molecular docking studies. By analyzing the binding interactions of these compounds with crucial *M. tuberculosis* targets, including key enzymes and protein receptors, we identified several compounds with notable binding affinities. The study highlights these natural products as promising candidates for further development and underscores the importance of exploring natural compounds in the search for new TB therapies.

T2- 0006

Linear Calibration-Dose Tuning Adjustment of X-Band Linear Accelerator in Accuary™ Cyberknife M6

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Abstract

Cyberknife M6 radiotherapy treatment machine having an X-band LINAC in which a compact LINAC is mounted on a robotic arm instead of using a gantry to hold the X-ray source. It uses 9.3 GHz X Band accelerator which provides 6 MV photon beam energy with dose rate of 800 MU/min which enables to precisely irradiate small tumor area with high dose-rate non-coplanar beams.

This beam tuning procedure allows you to calibrate and adjust the LINAC dosimetry system, nominal dose amounts are delivered for MU value ranging from 10 to 200 using a fixed collimator opening and measuring the dose detected.

X-Band LINAC is calibrated for a range of MU's instead of calibrating with a single larger MU value in case of conventional S-Band LINAC. Since it is used for SRT and SBRT hypofractionated treatments where high dose per fraction are delivered with high precision and every small dose counts, thus it is important to maintain the MU-Dose linearity and MU stability especially for smaller MU values for a beam delivering with high dose rate.

When delivering smaller MU with high dose rate having high dose per pulse, the chamber should be sensitive enough so that the total ionization per pulse is produced instantaneously, the charge has collected and recombined before the next pulse arrives.

It's important to tune the monitor chamber to have linear output throughout the MU range of small to high while delivering every pulse in high dose rate.

T2- 0007

Comparison of Accuracy of Ray Tracing and Monte Carlo in Regions of Heterogeneity

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Abstract

Ensuring accurate dose calculation is essential for an effective radiation therapy, especially in heterogeneous areas, such as the lungs. The dose optimization and calculation algorithms play a crucial role in achieving this. The CyberKnife Robotic Radiosurgery system utilizes two such algorithms- Ray Tracing (RT) and Monte Carlo (MC). The RT algorithm, being a correction-based algorithm, takes into account the effective path length of the beam traversed through the lung volume and the related attenuation along the path. The MC algorithm, on the other hand, is capable of simulating the individual particles' trajectories across the heterogeneous regions. The treatment planning was performed in the Accuray Precision® 3.3.1.3[2] treatment planning system (TPS) for the CyberKnife M6 system. Treatment plans were created using RT algorithm for water-equivalent slab phantoms, both with and without Styrofoam (air equivalent material), the former indicating the presence of inhomogeneity. The same plans were recalculated with MC, while keeping the beam parameters unchanged. The setup is reproduced, the treatment plans are executed using CyberKnife M6 and point doses are measured at reference point for each plan using calibrated 0.6cm^3 farmer chamber. Measured doses are tabulated and compared with the planned dose obtained from the TPS. In homogenous medium the behaviour of RT and MC are comparable with a minimal difference of less than 0.5%. In heterogenous region, the deviation of more than 2% is observed when RT algorithm is used. The result highlights the better performance of MC algorithm in heterogenous as well as the homogenous medium.

T2- 0008

DNA in concentrated solution: Effect of monovalent and divalent cations

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Abstract

The cations neutralize the DNA's negative charge at the phosphate group and help in stabilizing the double helix structure. More than that, cations play a significant role in many biological processes, such as DNA compaction and folding mechanisms. These cations can trigger the conformation changes in the DNA structure. Our objective is to study the conformation changes in the 1-BNA due to the monovalent and divalent cations at different temperatures. We used the AMBER-22 tool to simulate the solution and analyze the conformational changes in DNA using the Curves+ package. Our findings show the difference in binding affinities of monovalent and divalent cations at the minor and major grooves and around the backbone of the DNA.

T2- 0009

Patient-Specific Dosimetric Verification Using TLD in HDR Brachytherapy for Cervical Cancer with an In-House Phantom

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Abstract

In high-dose-rate (HDR) brachytherapy for cervical cancer, patient-specific quality assurance (QA) is essential to ensure accurate dose delivery to the target while minimizing exposure to surrounding healthy tissues. This study focuses on patient-specific quality assurance (QA) for high-dose-rate (HDR) brachytherapy, which ensures dosimetric accuracy in treatment plans. We developed a solid phantom designed for QA, capable of accommodating central vaginal surface (CVS) applicators used in cervical cancer treatment. Thermoluminescent dosimeters (TLDs) were cross-calibrated with a farmer-type ionization chamber using a Krieger Phantom and inserted at key points such as the applicator surface, virtual rectum, and bladder in the phantom. Treatment plans were generated, and after dose delivery, TLD measurements were compared to treatment planning system (TPS) calculations for different vaginal cylinder diameters (2 cm, 2.5 cm, 3 cm). Results indicated that the dose deviations between TLD and TPS values were within ±10% for $CaSo_4$: Dy and ±7% for LiF: Mg, Ti. The study concluded that the developed phantom is suitable for patient-specific QA, effectively reducing dosimetric errors and enhancing treatment accuracy in HDR brachytherapy. This method offers a reliable solution for patient treatment delivery verification and dosimetric accuracy.

Keywords: HDR brachytherapy; Cervical cancer; Patient-specific QA; Thermoluminescent dosimeters (TLDs); In-house phantom; Dosimetric accuracy.

T2- 0010

Impact of Aperture Size Selection in Oligometastatic of Brain – Dosimetric Evaluation

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Abstract

The approach for collimator selection is vital in controlling the plan quality criteria of Stereotactic radiosurgery (SRS). CyberKnife® Robotic Radiosurgery System(M6) delivers beam in 3D workspace unlike 360-degree rotation of the conventional Linear accelerator-based SRS treatment system. Different approach for aperture size selection for the treatment of brain metastasis is evaluated. Accuray Precision® 3.3.1.3[2] Treatment planning system provides multiple options for the collimator selection. Plans created for 3 PTVs which are separated more than 50mm apart. First approach used individual cone selection (7.5 mm and 10 mm) for each PTV, second one used combined PTV volume for cone size selection (12.5 mm, 30 mm, 50 mm) and in the third approach combined PTV with minimal cone opening (7.5 mm and 10 mm) which is derived from first approach. Plan created using Volo optimization algorithm. Plan evaluation criteria include delivery system parameters Total MUs, Number of Nodes, Beams, and dosimetric parameters like Conformity Index (CI), Homogeneity Index (HI), Volume receiving 2% and 98% dose (D2% and D98%), volume of 30% isodose line for spillage, percentage of isodose prescription and PTV maximum and minimum (D_{max},D_{min}) dose. The treatment time is considerably reduced when using the higher aperture size and spillage volume increased. Plans with optimized collimator size gives CI closer to unity and lower spillage volume ($V_{30\%}$ Isodose line). Lower prescribed isodose line in larger collimator opening and higher prescribed isodose line in smaller collimator opening is observed. The plan selection criteria are derived from As Low As Reasonably Achievable and the total treatment delivery time in accordance with the clinical goals. Wise selection of the cone size will help in the effective planning of SRS.

T2- 0011

Investigation of Red Blood Cell Microcirculation Using the DLVO Theory

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Abstract

During the study of blood microcirculation, some features were discovered that set it apart from Newtonian and non-Newtonian fluids. The laws of hydrodynamics or rheology alone cannot explain those peculiarities. In blood vessels with a diameter of more than 300 μm, the viscous incompressible fluid model works well; And when examining capillaries with a diameter of less than 300 μm, abnormal properties of blood flow appear, the study of the physical basis of which is still relevant today. In this article, blood is considered a multiphase physicochemical system. It is presented as a suspension of formed elements in plasma. Blood cells are an electrical system: the electrical properties of erythrocytes are expressed not by the magnitude of elementary charges but by the zeta potential - the electric potential at the boundary of the two phases - the erythrocyte and plasma. The study examined blood microcirculation, considering using the DLVO theory. A quantitative assessment of the flow of red blood cells in capillaries is given using resistance forces, hydrodynamic pressure, and coefficients of change in electrical potential. According to the results obtained, it can be seen that the discussed mechanical and electrical parameters have a significant impact on blood microcirculation. These factors influence the membrane of erythrocytes when moving in small capillaries and induce a gradient of electrostatic force in the direction of movement of red blood cells.

U1- 0001

Characterization & developmental analysis of Nano-Route Based Synthetic Red Blood Cells Using Biomaterials and Carbon Nanotubes – Prototype development using nanotechnology

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Abstract

This paper gives a brief abstracted overview on the final year project work that was carried out by the student under the guidance of the supervisors. Blood transfusion plays a critical role in modern healthcare, but the availability of safe and compatible blood for transfusion is often limited. Synthetic red blood cells (RBCs) have emerged as a potential solution to address this challenge. This abstract provides an overview of the development of synthetic RBCs as a promising alternative to natural RBCs. In addition, steps taken toward the development of artificial blood technology and some of their promises and hurdles will be highlighted. Synthetic RBCs are designed to mimic the structure and function of natural RBCs, allowing for effective oxygen transport and circulation within the body. They are typically composed of biocompatible materials that offer enhanced stability, extended shelf life, and compatibility with various blood types, minimizing the risk of adverse reactions during transfusion. On the membranes of these cells are proteins that the body recognizes as its own. For this reason, a person can use only blood that is compatible with her type. Currently, artificial blood products are only designed to replace the function of red blood cells. It might even be better to call the products being developed now, oxygen carriers instead of artificial blood. Oxygen and carbon dioxide throughout the body. They are also responsible for the typing phenomena. On the membranes of these cells are proteins that the body recognizes as its own. For this reason, a person can use only blood that is compatible with her type. Currently, artificial blood products are only designed to replace the function of red blood cells. It might even be better to call the products being developed now, oxygen carriers instead of artificial blood. Despite the advancements in science and technology, challenges remain in the development of synthetic RBCs. Achieving long-term stability, optimal oxygen-carrying capacity, and efficient removal from circulation after use are areas of active research.

Keywords – Blood, RBC, Nano, Simulation, Artificial, Nano.

U2- 0001

A Comparative Study of Technological Advancements from 5G to 6G

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Abstract

In this comparative study, the main technological evolutions are reviewed between 5G to 6G technologies in terms of frequency, spectrum and MIMO (Multiple Input, Multiple Output). The previous generation (5G) of mobile technology, brought about the capability for high-speed data transfer, low latency and even improved connectivity. The research describes the anticipated enhancements such as data rate, network capacity, energy efficiency and security. It also looks at the emerging use cases for 6G, encompassing immersive XR, holographic-type communications in real-time and end-to-end autonomous systems. This study also analyses the potential of 6G systems, but it also speaks to other critical issues around 6G that includes requirements for sustainable architecture, an advanced level of security and global standardization. The comparative analysis is expected to give a full picture how differently 6G can be from its predecessor, with highlighting the revolutionary capability of 6G in building up highly connected and intelligent world.

Keywords: AI Integration, 5G, 6G, Smart Technologies, Wireless Communication

U2- 0002

Deflection of light rays in electric field

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Abstract

Deflection of a light ray in a gravitational field, though as predicted by the general theory of relativity, occurs in the absence of any accompanying mass, suggesting that there is a scope for the light ray to deflect in an electric field without any electric charge accompanying it. This paper takes into account this and first discusses how the electric force mutually arises. From this it becomes clear that the electric force arises from the interaction of two electric fields in which electric charge plays no role. Because a light ray has an electric field, another electric field can apply a force on it, changing the direction of travel of the light ray. Again, since light rays have an electric field, if two light rays pass parallel and close together, an electric force also exists between them.

V2- 0001

Improvement of Leakage, Magnetic and Magnetodielectric Properties in Cobalt doped Gallium Ferrite

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Abstract

Gallium Ferrite is a magnetoelectric material, capturing growing attention due to its strong magnetoelectric coupling at room temperature. However, the application of the material in practical use is hindered due to its high leakage. In this work, the effects of cobalt (Co) substitution at the iron (Fe) sites of $GaFe_{1-x}Co_xO_3$ ($0.0 \leq x \leq 0.1$) polycrystals on the structure, electric and magnetic properties are investigated in detail. 5 at. wt.% substitution ($x = 0.05$) with cobalt ions achieves a reduction in leakage current density by four orders of magnitude due to reduced hopping between Fe^{3+} and Fe^{2+} ions and suppression of the oxygen vacancy formation. This is supported by higher dielectric constant and lower dielectric loss, as well as a significant difference between grain and grain boundary resistances. Two-phase-like magnetic behavior in magnetic hysteresis loop with enhanced magnetization and two magnetic transition temperatures are observed in the doped samples. All samples exhibited an increase in the magnetodielectric factor, indicating enhanced coupling between magnetic and electrical parameters. By concurrently increasing dielectric, magnetic, and coupling between them, this study describes a viable technique for lowering the most significant impediment to Gallium Ferrite's usage as a magnetoelectric device.

V2- 0002

Spin injection from a spin gapless semiconductor Heusler alloy into p-Si via MgO tunnel barrier and giant TMR in MTJ devices

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Abstract

In recent years, spintronic-devices have acquired much attention among the researchers all over the world since they have the capability of providing several exceptional-features such as ultra-low-power consumptions, nonvolatility, and reconfigurable-logic-functions. Although half-metallic-ferromagnets are recognized as the first choice of materials used for spintronic-device -applications, very recently, an exceptional class of spin-gapless-semiconductor (SGS) materials which exhibits a zero-gap for one spin-channel and a non-zero finite-gap for the other spin-channel, emerged to be one of the promising candidates in the field of spin-based-electronics. We report here fabrication of a high-quality exchanged-biased trilayer-magnetic-tunnel-junction (MTJ) utilizing a magnetron-sputtering-system. The MTJ is composed of a type-II spin-gapless-semiconductor Ti_2CoSi inverse Heusler-alloy, a thin MgO tunnel-layer and a half-metallic-ferromagnet Co_2MnSi Heusler-alloy. Spin-dependent-transport properties reveal that the micro-fabricated MTJ can act as a reconfigurable-magnetic-tunnel-diode, which lets the electric current to flow in either the forward or reverse-path relying on the relative alignment of the magnetization-direction of the upper and lower magnetic-electrodes. A considerably high on/off current ratio($\sim 10^3$) and a significantly low turn-on-voltage (V_T=0.09V) have been achieved at 5 K for both parallel and antiparallel configurations. Another important characteristic of our MTJ is that it exhibits extremely large tunnel-magnetoresistance-ratios of 892% at 5 K and 197% at room-temperature, which brings to light the utmost-importance of using the combination of HMF and SGS materials as magnetic-electrodes in a tunnel junction for modern spintronic-devices. All these exceptional features can undoubtedly nominate CMS/MgO/TCS MTJs as a promising candidate to serve as memory or logic-elements in next-generation ultra-high-density magnetoresistive-random-access-memories together with contemporary spin-based-electronic-devices.

V2- 0003

Dielectric and Impedance studies of Nano-composites of Ferrites substituted Ferroelectric $BaTiO_3$

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Abstract

Nano-composites of ferrites substituted in the ferroelectric $BaTiO_3$ with general chemical composition $0.3MFe_2O_4+0.7BaTiO_3$ (here, MFe_2O_4 = $Mn_{0.5}Zn_{0.5}Fe_2O_4$, $Mg_{0.25}Cu_{0.25}Zn_{0.5}Fe_2O_4$ and $Ni_{0.7}Co_{0.1}C_{u0.2}Fe_2O_4$) were synthesized using a hybrid synthesis technique which involves auto-combustion method followed by a mechanical grinding using the mixtures of ferroelectric phase component $BaTiO_3$ (BTO) and a magnetic(s) phase component which is ferromagnetic in nature. Presence of two phases in the nano-composites was probed using the powder X-ray diffraction (PXRD) studies, which confirms their crystalline phase. Peaks observed in the XRD spectrum indicated spinel cubic structure for the mentioned ferrites and tetragonal perovskite structure for BTO and, both spinel and tetragonal pervoskite structures for the synthesized nanocomposites. Surface morphology of the samples has been investigated using Field Emission Scanning Electron Microscope (FESEM), which reveals a good mixing of the two phases. The variation of dielectric constant and dissipation factor and impedance studies as a function of frequency at room temperature from 100 Hz to 1 MHz were carried out using a Hioki LCR Hi-Tester (3250-50). Dielectric constant found to decrease rapidly in the low frequency region and became almost constant in the high frequency region. Electrical conductivity and impedance parameters were deduced from the measured dielectric data has been thoroughly analyzed and found that the conduction mechanism in these composites is in conformity with electron hopping model.

Keywords: Ferrite; Ferroelectric; Phase; Composites.

V2- 0004

Polaronic Variable Range Hopping Mediated Electrical Transport Mechanisms in Ferromagnetic Pr_2FeMnO_6

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Abstract

The electrical transport properties of oxides are predominantly influenced by the interactions between electrons and phonons, leading to the formation of polarons, which govern the conduction mechanism. In perovskite oxide Pr2FeMnO6(PFMO), resistivity (ρ) exhibits insulating behavior at room temperature with ρ ~ 4.1 x 10^3 Ωm, consistent with previous reports. As the temperature decreases, ρ increases significantly, reaching 73.47 x 10^3 Ωm at 122 K, with an abrupt rise observed below 160 K. To explain the conduction mechanism, the Variable Range Hopping (VRH) model is employed. In this model, electron hopping between non-nearest neighbor sites occurs when the thermal energy is insufficient for hopping to nearest neighbors, favoring sites with smaller potential differences. The temperature dependence of resistivity from 2 K to 300 K fits well with the VRH model, as confirmed by a linear fit of the ln ρ vs. $1/T^{1/4}$ plot. The density of localized states at the Fermi level is calculated as N(EF) = 17.57 x 10^{-25} $eV^{-1}m^{-3}$ using the decay length (5.89 Å) of the localized wave function, which corresponds to the average Fe-Mn cation distance. The activation energy (E_a) varies from 0.13 eV at 122 K to 0.26 eV at 300 K, indicating the role of thermal activation in the conduction process. These results provide insights into the conduction mechanisms of PFMO in the context of electron-phonon interactions.

V2- 0005

Cation Distribution in the Spinel Oxide MnFe2O4: Magnetic and Raman Spectroscopy Study

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Abstract

MnFe2O4 is a remarkable magnetic spinel oxide whose crystal structure and magnetization can be tuned by the sample preparation conditions and chemical composition. In this study, a single phase polycrystalline $MnFe_2O_4$ spinel oxide (cubic, Fd-3m) was synthesized via solid-state reaction. Spinel structure (Space group Fd-3m) of MnFe2O4 has been confirmed through Rietveld refinement analysis and Raman spectroscopy. The cationic distribution in MnFe2O4 was identified as (Mn0.85 2+Fe0.153+)Tetra(Mn0.15 2+Fe1.853+)OctaO42−using the X-Ray diffraction data. EDX analysis confirms the sample composition. Magnetization vs temperature obtained in a field of 1 kOe reveal a high-temperature paramagnetic state to a collinear ferrimagnetic phase with TC = 561 K, θP = 580 K, an μeff=8.3 μBf.u. ⁄Magnetic susceptibility in the paramagnetic region is well explained by Neel's two-sublattice model.

W1- 0001

A review on orthopedic biomaterials: Properties, Advances, and Future Directions

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Abstract

Orthopedic biomaterials play a pivotal role in advancing fracture fixation, joint replacement, and dynamic stabilization within orthopedic applications. Primarily composed of metals, these biomaterials exhibit outstanding properties including high strength, ductility, fracture toughness, hardness, corrosion resistance, durability, and biocompatibility. Despite their versatility, the landscape of orthopedic implant materials remains dominated by a limited range of metals, ceramics, composites, and polymers. However, the durability of these implants is challenged by biological reactions and material degradation caused by wear and electrochemical corrosion. This review article underscores the imperative for advancing biomaterial development across dental and orthopedic applications. It discusses various types of biomaterials and their inherent properties, emphasizing the critical need for improved materials. Enhancing biomaterial design requires a comprehensive understanding of implant degradation mechanisms and their biological implications. The methods used to prepare biomaterials are detailed, including advancements in enhancing the surface biocompatibility of metal materials through techniques such as surface treatments and coatings. It critically examines current limitations in these approaches and proposes future research directions aimed at optimizing their effectiveness. By addressing these challenges, this paper aims to catalyze innovations that will lead to more durable and biocompatible biomaterials for both dental and orthopedic implants.

X2- 0001

Compression of super-Gaussian laser beam in plasma having relativistic nonlinearity

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Abstract

A study of the compression of super gaussian laser beam in plasma having relativistic non-linearity has been presented. A mathematical model having super-gaussian profile is investigated for the propagation of intense laser pulse in plasma. With the assumption that the relativistic nonlinearity dominates over other nonlinearities in plasma, this model has been formulated. A set up has been arranged having properties of self-compression and self-focusing and solved by a semi-analytical method. This result shows that by effect of diffraction of the laser pulse, group velocity dispersion, and non-linearity of the medium the pulse and beam width parameter of pulse gets focused at a different normalized distance.

X2- 0002

Effects of temperature on the space charge limited flow of a non-neutral plasma diode

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Abstract

A theoretical investigation is done on the steady states of a planar plasma diode where cold and stationary ions uniformly occupy the inter-electrode region. A purely monochromatic electron beam of constant temperature is injected from the emitter plate, and the emitted electrons are carried to the collector plate. The effects of finite electron temperature on the time-independent states are explored through a one-dimensional fluid-Maxwell's equations for arbitrary values of the neutralization parameter. Using the emitter electric field as a characteristic parameter, the steady-state solutions are visualized through the "Bursian" and "Non-Bursian" branches in "emitter electric field vs diode gap" parametric space. It is found that finite electron temperature modifies the space charge limit. The value of maximum attainable steady state current decreases with increasing temperature.

X2- 0003

Terahertz Radiation Generation through Cylindrical Nanoparticles

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Abstract

This paper presents an analytical model for terahertz (THz) radiation generation from cylindrical nanoparticles (CNPs) under laser excitation. Cylindrical nanoparticles exhibit radiation generation due to their distinct electronic and optical properties. Their strong interaction with laser fields significantly enhances nonlinear optical effects, which are crucial for efficient THz radiation generation. Additionally, this study focuses on the influence of their geometric parameters on the amplitude of THz radiation produced by these nanoparticles. The results provide valuable insights into optimizing the design and geometry of cylindrical nanoparticles for improved THz radiation generation, contributing to the development of compact and efficient THz sources.

Keywords: THz Radiation, Cylindrical Nanoparticles, Laser Excitation, Nonlinear Optical Effects.

Y2- 0001

Simulation Studies of Tissue Equivalent 3-D Fricke Gel Dosimeter for Stereotactic Radiotherapy

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Abstract

Stereotactic radiosurgery (SR) can be used to treat cancer, epilepsy, trigeminal neuralgia and arteriovenous malformations in different human organs, like the brain, spine with the help of radiation dose to the defective cells. Therefore, dose-verification techniques and specific quality assurance programs for routine radiation treatments having appropriate dosimetry equipment with end-to-end 3D dose verification capabilities are required. Out of different 3D dosimetry systems, hydrogels have emerged as innovative soft materials with widespread applications in drug delivery, tissue engineering, and gel dosimetry. The best technique used to measure the Percentage Depth Dose is the Monte Carlo simulation (MC). There are many different applications of MC but in medical physics it would be to simulate radiation transport. Synchrotron SR consists in loading the tumor with a high atomic number element, and exposing it to monochromatic x-rays from a synchrotron source. The dose distribution results from both the x-ray irradiation and the presence of the element, proportional to the absorbed dose. In this work, phantoms of dimension 100x100x100 cm^3 made of Fricke gel, hydrogel matrices based on PVA chemically cross-linked with Glutaraldehyde with chelating agent Xylenol Orange, were considered through which different dose was given from a x-ray source at a distance 100 cm from phantom. A 10 cm thick tungsten collimator block was placed between the source and the target to obtain a radiation field of 10x10 cm^2 at the target surface. Simulation was performed with the help of GEANT4 and the responses were reported.

Keywords: Stereotactic radiosurgery, Fricke gel, 3D dosimetry, GEANT4

Y2- 0002

Study of terrestrial gamma radiation and its health implications in the coal mining areas of Assam

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Abstract

The study assesses gamma radiation levels in two coalfield regions of Assam, namely Dilli-Jeypore and Makum coalfield, using a Micro-R Gamma Survey Meter (UR705). The key parameters calculated include the indoor and outdoor gamma dose rates (IGDR, OGDR), annual effective dose equivalent (AEDE) and excess lifetime cancer risk (ELCR). In Dilli-Jeypore, both AEDE and ELCR slightly exceed global standards, while in Makum, they are significantly higher than recommended levels of 0.48 mSv y-1 and 1.45×10-3, respectively. Long term exposure to elevated radiation levels, as observed in both regions, increase the likelihood of radiation-induced health effects. This study highlights the significance of addressing environmental radiation exposure in coalfield regions and the need for radiation monitoring and mitigation efforts to reduce health risks for the local population.

Y2- 0003

A Study on propagation of Electromagnetic waves

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Abstract

The propagation of electromagnetic waves in various media is studied. Waves of this type (radiation waves) from the far-field part propagate as they are accompanied by changes in electric field, magnetic vector potential or coupling fields over distances directly related to wavelength and further exposed for detection. Reflection, refraction, diffraction absorption and scattering are the main propagation mechanisms which change wave behavior transmission efficiency. Electromagnetic wave propagation is crucial in various fields including communication, medical imaging, remote sensing and endless industrial technologies etc. It serves an essential role both for scientific understanding and practical development. The electromagnetic waves propagate is critical other than in some applications of modern radios systems, radar and more scientific problems. This manuscript attempts to bridge the gulf between highly theoretical treatments of electromagnetic wave propagation and practical commercial microwave engineering practice. Maxwell's equations are the basis for understanding wave propagation, and the authors provide a model how electric and magnetic fields interact. Reflection, refraction, diffraction and scattering phenomena are highlighted as the key factors that affect wave propagation in realistic environments. In the analysis, wave attenuation as well polarization and influences of terrain effects on waves, atmospheric conditions and ionosphere disturbances are considered. In particular, near-field and far-field and plane wave propagation models based on radiation modes are considered relative to propagating waves.

Key Words: Absorption, Electromagnetic Waves, Medium, Propagation, Scattering.

Y2- 0006

Study the characteristics of electric field inside the human head due to high Frequency EM waves

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Abstract

In the current world, the use of electronic gadgets like cell phones and Wi-Fi router is widespread. It is continuously exposing people to electromagnetic radiations. During the phone calls, the head is most affected organ by the emitted radiation. This study discusses the interaction of electromagnetic radiation with the head. The aim of this manuscript is to explain the propagation of electromagnetic waves through various tissues of head including the outer skin, skull, gray and white matter of the brain. When someone make a call, electromagnetic waves strike the outer layer of the head. The induced electric fields are partly reflected and transmitted by the tissue layers present in the human head. It is observed from graphs that the reflected and transmitted electric fields are decreased and increased respectively with increasing the velocity. A specific velocity of waves is observed in every tissue layer at which both the electric fields (reflected and transmitted) are equal. The equilibrium velocity is varied depending upon the dielectric properties of the biological tissues. The amplitude of the electric field and velocity of the transmitted waves are higher into the outer skin than other layer of body. The velocity and electric field are reduced as the waves travel through the bone, gray matter, and white matter of the head. These results contribute to understand the effects of EM waves on the human head and the propagation of electric fields through biological tissues.

Keywords: Electromagnetic waves, reflection, transmission, human head, propagation of EM waves.

Y2- 0007

Thermoluminescence Study of $NaLi_2PO_4$ Doped with Rare Earth Metal Dy^{3+} irradiated with gamma Ray.

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Abstract

Thermoluminescence is a form of luminescence exhibited by some materials which when absorb energy from electromagnetic radiation or other ionizing radiation, re-emits light upon heating of the material. These materials are used for the purpose of dosimetery in medical, physical applications. In the present study thermoluminescence study of $NaLi_2PO_4$ doped with rare earth metals Dy^{3+} is done using gamma ray. Comparative thermoluminescence study is done between these materials. Different concentration of dopants in these materials varying from 0.1% to 1% is studied and thermoluminescence study is done by analyzing different parameters using initial rise method, Chen's peak method. Dose range of gamma ray is varied from 10 gy to 15 Kgy. Linearity of these materials for different concentration of dopants for gamma ray is analysed.

Z2- 0001

Design, Development & Implementation of an IoT-Enabled Fire Alarm Circuit Applying Instrumentation Concepts using Optical Sensor Materials based Wireless Communication Physical Systems

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Abstract

Fire Alarm Circuit is a simple circuit that detects the fire and activates the Siren Sound or Buzzer. Fire Alarm Circuits are very important devices to detect fire in the right time and prevent any damage to people or property. Fire Alarm Circuits and Smoke Sensors are a part of the security systems which help in detecting or preventing damage. Installing Fire Alarm Systems and Smoke Sensors in commercial buildings like offices, movie theatres, shopping malls and other public places is compulsory. There are many expensive and sophisticated Fire Alarm Circuit in the form of stand-alone devices, but we have designed five very simple Fire Alarm Circuits using common components like Thermistor, LM358, Germanium Diode, LM341 and NE555.This is a very simple alarm circuit using Thermistor, LM358 Operational Amplifier and a Buzzer. The primary purpose of fire alarm system is to provide an early warning of fire so that people can be. evacuated & immediate action can be taken to stop or eliminate of the fire effect as soon as possible Alarm can be triggered by using detectors or by manual call point (Remotely). The research paper explores the integration of Internet of Things (IoT) principles and instrumentation concepts from physics in the creation of an advanced fire alarm circuit. The study focuses on leveraging IoT technology to enhance fire detection capabilities through smart and wireless communication. The circuit's design incorporates physics-based instrumentation concepts to ensure accuracy and reliability in fire detection. The research aims to contribute to the development of innovative solutions in fire safety by combining modern IoT approaches with fundamental principles from the field of physics.

Z2- 0002

Comparative study of various development board based on microcontroller

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Abstract

The embedded system is the combination of electronics hardware and software. Microcontrollers are essential components of embedded systems that enable various applications in different domains. However, choosing the most suitable microcontroller for a specific project can be challenging, as there are many factors to consider, such as architecture, peripherals, development environment, and application areas. In electronics market, numbers of embedded controller boards is available for engineers/developers to utilize it on basis of requirement and functions. The vision of this paper is to compare various controller boards through their input/output port capacity and communication method as well as capability of interconnection with each other. It will help to engineers and professional developers to easily choose their microcontroller to develop any embedded system.

Z2- 0003

Design Optimization of Compact Microstrip Patch Antenna for 5G Networks

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Abstract

Since the commencement of the progression toward the next generation of communication systems, an explosive exploitation of the millimeter waveband/millimeter band has been observed. Since 5G systems are currently of utmost relevance in the present telecommunication scenario, this paper is penned with the goal to introduce a rectangular microstrip patch antenna capable of operating in the millimeter band frequency with an operational frequency of 42.6 GHz with an appreciable gain of 6.41 dB, a VSWR of 0.6, and a return loss of -28.71 dB, along with a radiation efficiency of 97%. The paper contains the design parameters as well as the results obtained from the proposed antenna simulation conducted utilizing the HFSS software.

Z2- 0004

Design and Performance of a Dual-Band Planar Dipole Antenna frEnhanced Connectivity

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Abstract

In the proposed antenna design, a microstrip patch antenna with dual-band characteristics was designed using a combination of meander lines. The planar dipole antenna (PDA) operates at 17.6 GHz with a return loss of -20.69 dB with a gain of 3.55 dB and at 8 GHz with a return loss of -22.65 dB and a realized gain of 1.63 dB. This versatile high-performance antenna maintains reliable communication performance by switching to a lower frequency when necessary, ensuring connectivity, effective spectrum management, and resilience against interference. Its capability to provide backup links and alternative frequencies enhances service availability for broadcasting, telecommunication, data transmission, and remote sensing applications.