Abstract Book of

4th International Conference on Condensed Matter & Applied Physics

ICC 2023 October 09-10, 2023



Editors:

Dr. Bhuvneshwer Suthar Government Dungar College, Bikaner

Dr. M. S. Shekhawat Engineering College, Bikaner

Dr. Sudhir Bhardwaj

University College of Engineering & Technology, Bikaner

Organized under joint auspicious of

Condensed Matter Research Society (CMRS) & Department of Physics, Engineering College, Bikaner

World Science Publications, Bikaner, India

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ISBN: 978-81-966113-0-9

Publisher:

World Science Publications, Bikaner

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www.iccindia.in

PREFACE: ABSTRACT BOOK OF ICC 2023

It is with immense pleasure and a profound sense of accomplishment that we welcome you to the 4th International Conference on Condensed Matter and Applied Physics (ICC 2023). This event marks the continuation of a remarkable journey that began with our inaugural conference and has flourished over the years, thanks to the unwavering faith and support of our dedicated participants and delegates.

The success of the previous three conferences in this series has been a testament to the vibrant community of researchers, scientists, and scholars who share a passion for advancing the frontiers of condensed matter and applied physics. Your enthusiasm and commitment to scientific excellence have driven us to organize yet another exciting gathering.

ICC 2023 is organized under the joint auspices of the Condensed Matter Research Society, Bikaner (CMRS), and Engineering College, Bikaner. It will take place on October 9-10, 2023, providing a platform for researchers from around the world to converge and share their groundbreaking work.

This year, we received an overwhelming response, with over 400 contributory papers submitted. These papers reflect the depth and breadth of research in the field, covering a wide array of topics and pushing the boundaries of our understanding of condensed matter and applied physics.

In addition to the contributory papers, we are proud to host the Young Achiever Award (YAA), which recognizes the outstanding contributions of emerging researchers. Eight young and promising participants have been nominated for this prestigious award, and we look forward to celebrating their accomplishments.

Furthermore, ICC 2023 boasts an impressive lineup of speakers. We have the privilege of hosting ten distinguished invited speakers, each bringing their unique perspective and insights into the world of condensed matter and applied physics. Additionally, two keynote lectures will offer a broader view of the current state and future prospects of these fields.

As we embark on this exciting journey of scientific exploration and collaboration, we extend our heartfelt gratitude to all the authors, reviewers, participants, and supporters who have made ICC 2023 a reality. Your dedication and enthusiasm are the driving forces behind this conference's success, and we are deeply appreciative of your contributions.

We hope that ICC 2023 will not only be a platform for sharing knowledge but also a source of inspiration for all participants. It is our sincere wish that the interactions and discussions during this conference will lead to new discoveries, collaborations, and innovations that will shape the future of condensed matter and applied physics.

Once again, welcome to ICC 2023. Let us come together to celebrate the wonders of condensed matter physics and the applications that drive progress in our world.

October 09, 2023

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Programme Schedule

of 4th International Conference on Condensed Matter & Applied Physics

Day 1 – Monday, 09 October, 2023

8:00 AM - 9:00 AM **Registration & Breakfast**

9.00 AM - 9:30 AM Inaugural Ceremony

9:30 AM - 11:00 AM **Key Note Lecture**

Session Chair: Prof. Sampad Kumar Biswas, Department of

Metallurgical & Materials Engineering, MNIT,

Jaipur

Session Co-Chair: Prof. Narendra Bhojak, Department of

Chemistry, Govt. Dungar College Bikaner

Keynote Lecture -1: Prof. J V Yakhmi, Ex Associate Director, BARC,

Mumbai

Keynote Lecture -2: Dr. Michele Di Lauro, Ialian Institute of

Technology, Italy

Keynote Lecture -2: Prof. Sampat Raj Vadera, Indian Institute of

Technology Jodhpur, Jodhpur

11:00 AM - 11:30 AM High Tea

Session Chair: Prof. J V Yakhmi, Ex Associate Director, BARC,

Mumbai

Session Co-Chair: Dr. Ravindra Mangal, Ex. VC. Global National

University & Principal Govt. College, Nokha

Invited Lecture -1: Prof. Vivek Kumar Gupta, Department of

Physics, University of Jammu, Jammu

Invited Lecture -2: Prof. Sampad Kumar Biswas, Department of

Metallurgical & Materials Engineering, MNIT,

Jaipur

Invited Lecture -3: Dr. Atiar Rahaman Molla, CSIR-Central Glass &

Ceramic Research Institute

Invited Lecture -4: Prof. Narendra Bhojak, Department of

Chemistry, Govt. Dungar College, Bikaner

1:30 PM -2:00 PM	Lunch		
2:00 PM -3:30 PM	Poster Session –I (c Parallel Oral Session		(A1-All, B1-0007 to B1-0047)
		IA	(A1-0002 to A1-0038)
		IB	(A1-00048 to A1-0085)
		IC	(A1-0087 to A1-0108)
		ID	(B1-0010 to B1-0038)
3:30 PM - 4:30 PM	YAA Paper presen	tation	
	Session Chair:	Dr. Micl	nele Di Lauro, Ialian Institute of
		Technol	ogy, Italy
	Session Co-Chair:	Prof. Aja	ay Nagar, Department of Physics, Govt.
		Dungar	College Bikaner
4:30 PM - 4:45 PM	Tea Break		
4:45 PM - 6:15 PM	Poster Session -II (offline)	(B1-Rest, C1, D1, E1, F1-All)
	Parallel Oral Sessi	on (online)
		IIA	(B1-0040 to B1-0062)
		IIB	(B1-0064 to B1-0086)
		IIC	(B1-0089 to B1-0102)
		IID	(C1-All)
7:00 PM Onwards	Dinner		

Day 2 – Tuesday, 10th October, 2023

6:00 AM Well Renowned Deshnok Temple Visit

8:00 AM - 8:30 AM Morning Breakfast 8:30 AM - 10:30 AM Invited Session-II

Session Chair: PROF. VIVEK KUMAR GUPTA, Department of

Physics, University of Jammu, Jammu

Session Co-Chair: PROF. ANAMI BHARGAVA, Govt. Dungar

College, Bikaner

Invited Lecture -5: PROF. DR. OSMAN ADIGUZEL, Firat

University, Elazig, Turkey

Invited Lecture -6: DR. VINCENT MATHEW, Department of

Physics, Central University of Kerala,

Kasaragod, Kerala

Invited Lecture -7: DR. NAVEEN K ACHARYA, Faculty of

Technology & Engineering, The M. S. University

of Baroda, Vadodara

Invited Lecture-8: DR. ANIL BARI, Arts, Commerce & Science

College, Bodwad, Maharashtra

10:30 AM - 11:00 AM High Tea

11:00 AM – 1:00 PM **Poster Session-III** (G1, H1, J1, K1, A2, B2, C2, D2, E2-All)

Parallel Oral Session

IIIA (D1, E1, F1, G1-All)

IIIB (H1,I1,J1-All) IIIC (K1,A2,B2-All)

IIID (E2-All)

1:00 PM-2:00 PM Lunch

2:00 PM-3:30 PM Invited Session-III

Session Chair: Prof. G P Singh, Ex-principal, Govt. Dungar

College, Bikaner

Session Co-Chair: Prof. M D Sharma, Govt. Dunagr College Bikaner

Invited Lecture -9: Prof. RAJENDRA SINGH JADEJA, Maharaja

Sayajirao University of Baroda, Vadodara

Invited Lecture -10: DR. Nilesh Ugemuge, Anand Niketan College,

Warora, Chandrapur, India

Invited Lecture-11: Dr. M V Reddy, Energy Storage Echnology (New

graphite world) (NMG), Quebec, Montreal,

Canada

3:30 PM - 4:30 PM **Oral Session**

Session Chair: Dr. Nilesh Ugemuge, Anand Niketan College,

Warora, Chandrapur, India

Session Co-Chair: Prof. Smita Sharma, Govt. Dunagr College

Bikaner

4:30 PM - 5:00 PM **Valedictory Session**

5:00 PM **Tea**

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Keynote Lecture 1

Points to Ponder for success in scientific research

J.V. Yakhmi Ex Associate Director, BARC, Mumbai

This talk will discuss multidisciplinary topics of research which hold promise for useful applications. They are mostly on the interface of NBIC (Nano-, Bio-, Info- Cogno-). Examples will be discussed from author's own work in the past on molecular magnets and superconductors. New topics to be highlighted are wheel-free motion, self-assembly, soft matter, bistabilty, materiomics, growth of nanocrystals for sensors, etc. Besides, hints will be provided to young researchers for acquiring skills useful for career growth.

IT-001

Disorder in the organic molecular crystals

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Abstract. Crystal structure determination by X-ray diffraction has become a standard analysis in chemical research. While the quality and efficiency of the equipment has improved considerably over the past years and decades and while the power of programs and computers has made remarkable progress in that same period there has remained one domain where crystallographers still spend lots of their time, and this is when the structures under investigation are disordered. Disorder is a physical phenomenon leading to uncertainty in the chemical composition, or in the spatial arrangements of atoms. The disorder of some atoms may cause conformation difference for molecules. Disorders sometimes reveal themselves only atom-by-atom. In real crystals, as the arrangement varies only somewhat in different unit cells, disorder does not seriously affect the refinement of crystal structures. However, if the arrangement is significantly different from one-unit cell to another, the structure is probably disordered. In practice, disorder shows up much later at the refinement stage. The refinement programs have constraints and restraints to handle a wide range of disorder. It refines disorder by dividing the disordered atoms into groups. The shape and size of the thermal ellipsoids is one of the most important indicators for problems with the molecular model. Amongst the difficulties to refine disorders is the fact that the bond length to the environment may vary resulting in bad displacement parameters. For resolving disorder in molecules, basic chemical knowledge and an understanding of the fundamentals of crystallography is as important as patience, intuition and the skilful use of constraints and restraints. The answer to the question of whether a specific disorder is worth refining is as much based on experience as the assessment of data quality and difference density maps. Examples of successfully refined disorder in the organic molecular crystals will be presented.

IT-002

Large Deformation in Armor Ceramics under dynamic loading

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Abstract. Advanced ceramics like Alumina (Al₂O₃) Aluminum Nitride (AlN), Boron Carbide (B₄C), Silicon Carbide (SiC) etc. have been found to be candidate materials in protecting against high level projectile threat and reducing the weight of the armor. Ceramics are brittle in nature under quasistatic loading conditions. However, these ceramics can undergo substantial deformation by manifestation in the form of dislocation, stacking faults and twins leading to failure and compressive fragmentation. Inelasticity in ceramics is of fundamental importance in understanding the failure under dynamic loading. The present talk will deliberate on the deformation behaviour and its manifestation in microstructure for energy absorption in armor ceramics like Al₂O₃, AlN and SiC. Detailed microstructural investigation of the hot pressed SiC ceramics both before and after impact with bullet will be discussed. Analytical microscopy of recovered fragments after impact reveals high dislocation and stacking fault density in the polycrystalline grains which indicates a non-linearity in stress-strain behaviour at high strain rate.

IT-0003

Spearheading the Future of Display Technology with Strong, Transparent Nano-crystalline Glass-Ceramics

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Abstract. Display technology has witnessed remarkable advancements in recent years, with an increasing emphasis on strength, transparency, and durability. This paper delves into the revolutionary potential of strong, transparent nano-crystalline glass-ceramics in shaping the future of display technology. Specifically, we focus on the unparalleled strength offered by ion-exchanged glass-ceramics, surpassing conventional glass-based ion-exchange strengthened displays.

The unique properties of nano-crystalline glass-ceramics, combined with the ion-exchange process, enable the creation of display materials that are significantly stronger and more robust. Through controlled ion-exchange techniques, these glass-ceramics undergo a transformation that enhances their mechanical properties, making them highly resistant to impact, bending, and scratching. This breakthrough allows for the development of shatterproof displays, mitigating the risk of damage and improving user experience.

This paper will present synthesis of precursor glass and optimization of ceramization heat-treatment protocol exploiting crystallization kinetic studies for controlled crystallization of precursor glasses in order to produce nano-crystalline, high strength, transparent glass-ceramics. Further ion-exchange strengthening techniques will be discussed. In this paper it will be presented how scratch-resistant, high-strength, transparent nanocrystalline glass-ceramics (GC) can be produced which can outperform the traditional soda lime silicate (SLS)/lithium alumino silicate glass-based displays. Few examples of ion-exchangeable glass-ceramics will be presented to demonstrate the high potential of glass-ceramics for empowering nest-generation displays.

The implementation of strong, transparent nano-crystalline glass-ceramics in display technology showcases a promising shift towards reliable and durable screens. Their ability to withstand rigorous usage, coupled with desirable optical properties, positions them as frontrunners for next-generation displays. Moreover, their potential extends beyond consumer electronics, finding applications in automotive displays, wearable devices, architectural surfaces and even for vehicle armours.

IT-004

Thermomechanical Processes and Crystallography of Reversibility in Shape Memory Alloys

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Abstract. Metals and many alloy systems have different phases at different conditions, and these phases are described in phase diagrams as alloy composition-temperature or composition-pressure space. A series of alloy systems exhibit a peculiar property called shape memory effect in β -phase region. These alloys are called shape memory alloys and they are very sensitive to external conditions This phenomenon is initiated with thermomechanical processes on cooling and deformation, and performed thermally on heating and cooling, with which shape of the materials cycle between original and deformed shapes in reversible ways. Therefore, this behavior can be called thermoelasticity. This is plastic deformation, due to the soft character of the material in low temperature condition, with which strain energy is stored in the materials and release upon heating, by recovering original shape.

Shape memory effect is governed by phase transformations in crystallographic level, 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 planes of austenite matrix, along with lattice twinning reaction, and ordered parent phase structures turn into twinned martensite structures. The twinned structures turn into detwinned martensite structures by means of

stress induced transformation with stressing the material in the martensitic condition. These reactions are driven by lattice invariant shear, and lattice twinning and detwinning reactions play important role at the martensitic transformations.

These alloys exhibit another property called superelasticity, which is performed with mechanically stressing and releasing the material in elasticity limit at a constant temperature in parent phase region and shape recovery occurs instantly upon releasing, by exhibiting elastic material behavior. Stress-strain profile exhibits nonlinear behavior at stress-strain diagram, stressing and releasing paths are different and hysteresis loops refers to energy dissipation. This phenomenon is also result of stress induced martensitic transformation and ordered parent phase structures turn into detwinned martensite structure with stressing.

Copper based alloys exhibit this property in metastable β -phase region. Lattice twinning and lattice invariant shear are not uniform in these memory alloys and gives rise to the formation of layered structures, like 3R, 9R or 18R depending on the stacking sequences on the $\{110\}$ - type close-packed planes of the parent phase. Unit cell and periodicity is completed through 18 layers in 18R structures in ternary copper-based alloys. Also, parent phases of these alloys have the high symmetry, and product martensitic phases have low symmetry at low temperature

In the present contribution, x-ray diffraction and electron diffraction studies were carried out on copper based CuZnAl and CuAlMn alloys. X-ray diffraction profile and electron diffraction patterns exhibit super lattice scattering. Critical transformation temperatures of these alloys are over the room temperature, at which alloy samples are completed in the martensitic state. These alloy samples were aged at room temperature, and a series of x-ray diffraction profiles and electron diffraction patterns were taken. X-ray diffractograms taken in a long-time interval show that scattering angles, peak intensities and characteristics change with ageing at room temperature. This result refers to the rearrangement of atoms in diffusive manner.

IT-005

Magnetogenetics, from present to future

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Abstract. Magnetogenetics is an approach that enables precise control over the biological functions of cells, groups of cells, tissues, and even organisms through the integration of magnetic fields and genetic engineering techniques. The clear advantages of magnetogenetics in potential clinical applications include the ability to remotely manipulate cell fate and gene expression by leveraging the interaction between cells and externally applied magnetic fields. This report aims to provide a conceptual outline of our current understanding of key aspects of magnetogenetics and their relevance to human diseases, with the goal of informing the design of future studies. We discuss the effects of moderate to ultrahigh magnetic fields (uniform, gradient, low-frequency, and static magnetic fields) on various cellular aspects, including membrane ion channels, membrane potential, cell division, cytoskeleton perturbations in cells of diabetic mice, DNA synthesis in cancer cells, and lung cancer-bearing mice. Magnetogenetics holds promise for therapeutic applications. By selectively controlling cellular functions using magnetic fields, it may be possible to develop new approaches for treating various diseases, including neurological disorders, by modulating neural activity, delivering targeted therapies, or promoting tissue regeneration.

Acknowledgement: Project is funded from the Mobility Program budget of the Czech Academy of Sciences and the Chinese Academy of Sciences (CAS-23-01).

Light-Matter Interaction in Topological Photonic Systems

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Abstract. Photonics research is always concerned with innovative techniques to control light using optical structures. Recently, topological photonics has become a crucial framework for such investigations and continues to expand as a valuable source of new ideas for enhancing the performance of various photonic devices. The spectra of electromagnetic radiation in periodic media form band structures similar to the electronic energy band of condensed matter systems. Enlightened by the topologically nontrivial bands in the quantum system, topological photonics in its initial stage was focused on finding effects similar to the direct analogies of topological effects in the condensed matter systems. However, the bosonic nature of photons makes the photonic system distinct from its condensed matter counterparts. However, it provides platforms to study new effects, such as non-Hermition topology, which has no counterpart in an electronic system. This talk is aimed at providing an overview of the subject of topological photonics and its current level of applications.

IT-007

Transport Properties of Nanocomposite Piofgs Polymeric Membranes

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Abstract. Properties of nanocomposite polymers have recently been paid much attention due to their extensive applications in industrial research. Introducing inorganic nanoparticles in the polymer matrix alters the structure of the host polymer, which can improve separation properties. Another series of membrane materials i.e. thermally rearranged (TR) polymers and their composites have shown good combinations of gas permeability and selectivity in past few years. Polyimides containing orthopositioned functional groups (PIOFGs) have better applications for gas separation in contrast to conventional glassy PIs after thermally rearrangement. Introduction of nanoparticles into the polymer matrix has been shown to modify transport properties in polymeric membranes. It is proposed to examine the effect of thermal rearrangement on the nanocomposite polymer in contrast to the pure polymer. Transport properties of a thermally rearranged polyimide nanocomposite membrane compared with a neat thermally rearranged polymer membrane using H₂, CO₂, N₂, O₂ and CH₄ will be presented.

IT-008

Nanocrystalline Zinc Oxide: Synthesis, characterizations and their potential use as a sensor material

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Abstract. Nanocrystalline ZnO powders were synthesized using ultrasonic atomization technique. Effect of precursor concentration, pyrolysis temperature and aerosol carriers (Air/Oxygen) on ultrasonically atomized nanocrystalline ZnO powders was studied. The powders were characterized using X-ray diffraction, transmission electron microscopy, selective area electron diffraction, absorption spectroscopy and photoluminescence. It was observed that the powder consisted of nanocrystallites with sizes less than 20 nm. The nanocrystalline ZnO powder showed that crystallite sizes were observed to increase with an increase in the concentration of solution and pyrolysis temperature. The influence of air and oxygen on crystallite morphology was studied using TEM. It was confirmed from TEM analysis that the crystallites were nearly spherical in powder prepared in the presence of compressed air. In the presence of pure oxygen, the crystallites could acquire regular hexagonal shape. The effect of precursor concentration, pyrolysis temperature and aerosol carriers on crystallite size and morphology of nanocrystalline ZnO powders is reported in the present study. Furthermore, this nanocrystalline ZnO powder is used to prepared thick films using screen-printing techniques. Thick film is used as sensor to test the conventional gas (LPG, Carbon dioxide, Hydrogen, Ammonia, Ethanol and Chlorine) and simulant (Dimethyl Methyl Phosponate [DMMP], 2-chloroethyl phenyl sulfide [CEPS] and 2-chloroethyl ethyl sulfide [CEES]) of highly toxic chemical warfare agents (CWAs). The thick film sensor gives maximum response to Ammonia (conventional gas) and DMMP (simulant of CWAs).

IT-009

Synthesis and Crystal features of acylpyrazolone derived Inner transition metal complexes along with the study of covalency and physical parameters from their electronic and emission spectra

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Abstract. Acylpyrazolone are an exclusive kind of β -diketones that have drawn a lot of interest because of their variable 7 to 9 coordinated geometry, expansibility, acute and high absorption coefficient values, proficient Antenna effect, luminous probe activities, electrical, catalytic, and biological activities. Most lanthanide ions can display great absorption and emission characteristics, in which Lanthanide acylpyrazolone complexes possess distinctive properties due to its increased intensity, composition and symmetry of the coordination sphere, which illuminate their favoured application. Our laboratory is synthesizing various acyl pyrazolone derivatives, their Schiff bases and corresponding complexes with inner transition f-block elements (like U, Nd, Dy, Tb, etc.) with characterization using various spectroscopic techniques and also by single crystal x-ray diffraction. DFT, Hirshfeld and other computational methods are also used to get insight into the structure of these complexes. The attempt has been made to use these complexes to investigate the type and degree of covalency, extraction ability, Antenna effect energy diagram, oscillator strength, Judd-Ofelt parameters, covalency parameters, etc. from their electronic and solid-state emission spectra. The present talk is aimed to give highlight of the work going on in my laboratory on the acylpyrazolone derived Inner transition metal complexes.

IT-0010

Host sensitization of luminescence of lanthanide activators in Tungstate and Vanadate based Phosphors

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Abstract. Host sensitization of luminescence of lanthanide activators in different matrices like tungstate, vanadate, etc. plays vital role in many optoelectronic applications such as information storage, security, tunable solid-state lighting, laser materials and w-LEDs, etc. The sensitized emissions of Nd ³⁺ or Sm³⁺ were found to be much more efficient than a direct excitation of lanthanide ions (Ln³⁺). A comparison of estimated dipole-dipole energy-transfer rates with observations supports the importance of energy migration of the intrinsic excitations. The available tunable luminescent materials reported so far still suffer from several drawbacks of low efficiency or poor stability, thus restraining their further applications, efficient and stable lanthanide coordination polymers (LCPs) developed with tunable luminescence as a new option for optical multiplexing. Their multicolor emission from green to red and naked-eye-sensitive green emission with tunable lifetime can be controlled by host differential sensitization and energy transfer between lanthanide ions reported.

To achieve the noted advantages of host sensitized Ln³⁺ doped phosphors, we have studied, spectroscopic and luminescence properties of a series of NaBi(WO₄)₂ activated with trivalent lanthanides (Tb, Sm and Nd) and Nd³⁺ doped LiCa₃ZnV₃ O₁₂ prepared using the conventional solidstate reaction method. All samples were characterised by X-ray diffraction (XRD), scanning electron microscope (SEM) and photoluminescence (PL). The XRD study confirmed the tetragonal phase without any secondary phase. Particles of irregular shape ranging between 5 and 20µm were observed. Elemental composition was obtained from EDAX and results were found consistent with the formula. The formation of single-phase compounds was again confirmed through these results. Elemental mapping indicated that all elements were uniformly distributed. For NaBi(WO₄)₂:Tb, excitation was monitored for 545nm emission. Emission spectra upon excitation by 488nm showed prominent lines around 545 and 549 nm. These are due to the transition ${}^5D_4 \rightarrow {}^7F_5$. 5 mol.% Tb yielded maximum PL intensity. When 405nm excitation is used for Sm³⁺ doped phosphor, lines can be seen in three groups around 564, 600 and 647 nm. The highest emission intensity is observed for Sm³⁺ concentration of 5 mol.% and quenching was observed for high values. A weak band could be seen in the excitation spectra which is distinct from the f-f lines. The position of this band is close to that observed in the reflectance spectra. Hence it is proposed that there is host sensitization, even though weak, of the lanthanide luminescence in this host. Sensitization is most probably due to $Bi^{3+} \rightarrow Ln^{3+}$ energy transfer. Two types of emissions have been observed.

The self-activated luminescence could be observed in Nd^{3+} doped $LiCa_3ZnV_3O_{12}$ under UV excitation. The characteristic emission of Nd^{3+} is also observed. Apart from the f-f excitation, an efficient host sensitization of Nd^{3+} luminescence is observed. The $LiCa_3ZnV_3O_{12}:Nd^{3+}$ phosphor showed an intense Near Infrared emission at 1068nm due to the transition of ${}^4F_{3/2} \rightarrow {}^4I_{9/2}$, for 350nm excitation.

IT-0011

Thin and bulk Materials for Energy storage and Sustainability

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Abstaract. In recent years Advanced materials considerable interest in worldwide researchers due its interesting functional properties and applications in areas of energy, water, health care, and sensors. Research is being carried out worldwide to find alternative novel materials, improved the performance by various materials synthesis processes, surface modification, and fabrication technology.

In my talk, i will discuss thin and bulk nano oxide and nitride materials fabrication, physical properties, fundamentals, and applications related to Energy storage and conversion. Various chemical and

physical fabrication technologies for materials and its characterization techniques like Rietveld refined X-ray diffraction, Neutron diffraction, X-ray absorption spectroscopy, X-ray photoelectron spectroscopy, Rutherford Backscattering spectrometry, Scanning and Transmission electron microscopy (SEM/TEM), Raman/IR, density and BET surface area methods will be discussed. Importance of electroanalytical studies like cyclic voltammetry, galvanostatic cycling and impedance spectroscopy techniques for testing high performance evaluations, reaction mechanisms of energy storage materials and sustainability. Finally, I will discuss the challenges and opportunities for physics and basic sciences for future energy storage research.

Nanocomposite photocatalysts for wastewater treatment Suresh Sagadevan*

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Abstract. In recent years, the majority of people worldwide have been facing severe environmental pollution, resulting from the rapid development of science, technology, and industries. In addition, ecological problems and the energy crisis have become significant challenges for human beings, and extensive research needs to be conducted to maintain sustainability. In terms of the energy crisis and related concerns, electrical and solar devices made up of semiconductors and other photocatalysts are considered the most promising tools because they can be useful for the maintenance of the environment along with enhanced production of green energy. Therefore, various semiconductor photocatalysts have been widely applied in various fields, including photocatalysis and solar devices. However, the fast recombination of photogenerated carriers, low optical absorption, and small specific surface area greatly limit the performance of these photocatalysts. Photocatalysis is an environmentally friendly method that can be applied to degrade hazardous organic pollutants in wastewater. Owing to the limitations of conventional semiconductor oxide-based catalysts, especially in terms of limited applicability in the visible ultraviolet (UV) or solar regions, interest in the development of improved photocatalysts has increased in recent years. Photocatalysts, such as different nanocomposites, reduce the bandgap of single materials and also reduce the process of electron-hole recombination, giving higher efficacy for the application. Photodegradation typically increases with increasing catalyst loading, irradiation time, and reaction temperature, whereas a lower pollutant concentration is considered beneficial for photocatalysis. Different illustrations of nanocomposites, highlighting their potential use in wastewater treatment, have also been presented. It is generally observed that nanocomposites are better photocatalysts than pure nanoparticles, providing higher efficacies for pollutant removal.

YAA-0002

Fabrication of Flexible Supercapacitor using Nanostructured Conducting Polymer Composite H. Vijeth

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Abstract. Nickel oxide (NiO) is a promising electrode material in supercapacitor (SC) applications, but the poor electronic conductivity and weak electrochemical stability of NiO limits the fast charge/discharge rate and long-time reuse. Herein we report a core-shell nanostructure formed by NiO nanoparticles decorated on polypyrrole nanotube (PNT) through a chitosan (CS) layer (NiO/CS-PNT), as a supercapacitor electrode material. The PNT is synthesised using a self-degradable soft-template approach. The one dimensional (1D) nanotube structure gives increased surface area to polypyrrole (PPy). The inevitable aggregation of the NiO nanoparticles is reduced by the incorporation of CS, thereby increasing the surface area of the active material and bringing the higher electrochemical performance. NiO/CS-PNT core-shell nanostructure is found to have a large surface area, low charge transfers resistance (R_{ct}) and high specific capacitance (C_{sp}) as compared with that of NiO/PNT and pure PNT. Besides, an all-solid-state symmetric supercapacitor (SSC) was fabricated with NiO/CS-PNT as positive and negative electrode, which shows high power density (PD) of 4045.69 Wkg⁻¹ at an energy density (ED) of 27.80 Wh Kg⁻¹. Also, an outstanding cyclic stability was found with capacitance retention of 84.90 % even after 10000 cycles. The results demonstrate that the NiO/CS-PNT core-shell nanostructure is a favourable electrode material for supercapacitors.

Unusual Metallic Behavior at Low Temperature, High Pressure Structural and Thermoelectric Studies of δ – Ag₄SSe and TISe Single Crystals

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Abstract. Silver chalcogenide based superionic conductors possess liquid-like ionic diffusivity (10-3 $(\Omega.Cm)$ -1) which causes the variety of interesting physical properties such as, electronic topological transitions, metallization, and the possible emergence of superconductivity under pressure have attracted attention in recent years. Among these chalcogenides, Ag2S-Ag2Se solid solutions have been thoroughly investigated for several decades, due to many interesting high temperature optical, electrical, and thermoelectric properties exhibited. In view of this, we discuss our recent discoveries on Ag4SSe and TISe single crystal structural, high pressure behavior, electronic, magnetic and thermoelectric properties. The superionic electrical conductor Ag4SSe is reported to undergo an unusual first-order structural phase transition at ~260 K with concomitant anomalous electronic properties. The diamagnetic magnetic susceptibility is of larger magnitude in the low-temperature δ phase than in α -Ag4SSe. A diamagnetic susceptibility of larger magnitude is usually related to a lower density of states at the Fermi level which leads to a decrease in the Pauli paramagnetic susceptibility. Synchrotron based angle dispersive X-ray diffraction experiments have been performed on aguilarite-Ag4SeS, acanthite (α -Ag2S) type structure, up to \sim 20 GPa to probe its high pressure structural behavior. Our studies show that it undergoes two structural phase transitions at 2.6 GPa and at ~14 GPa to new high pressure phases, HP I and HP II respectively. Also, we discovered ultralow thermal conductivity in TlSe single crystal due to low energy optical phonon modes which strongly interact with the heat carrying acoustic phonons and they are associated with the intrinsic rattler-like vibration of Tl+ cations in the cage constructed by the chains of (TlSe2)nn.

YAA-0004

A Biosensor for the detection of Anemia Cancer using metal and defect multilayer 1D Photonic crystals

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Abstract. A one-dimensional photonic crystal-based biosensor has been designed for the diagnosis of anemia in a human with a defect layer of a blood sample. The proposed structure contains five periodic layers of semiconductors and a very thin defect layer of blood sample between two thin metal layers. Here the concentration of hemoglobin in red blood cells is helpful for the detection of anemia in a patient. The concentration of hemoglobin in a blood sample is a function of the refractive index. To analyze the transmittance properties, the thickness of a metal layer, angle of incidence, and refractive index/concentration of the defect layer have been varied by using the transfer matrix method. It has been observed that the proposed device contains a better quality factor and sensitivity in comparison to a simple structure.

Optimized Properties and Performance of All-inorganic CsSnI3Cl_{X-3} Absorber Layers for Flexible Perovskite Solar Cells

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Abstract. The growing energy need and rapid consumption of conventional energy resources motivated researchers to find feasible and cheap alternative resources. The wafer-based crystalline silicon photovoltaics is a commonly used solar cell technology, but it has high-cost and limited stock. Nowadays, perovskite solar cells (PSCs) have emerged as promising next-generation photovoltaic technology due to their low cost. A remarkable power conversion efficiency (25.7%) has been demonstrated for organic-based PSCs. Still, these are most degradable and less stable as the performance degrades rapidly because these perovskite materials decompose under ambient conditions [2]. Therefore, the instability of perovskites is a significant challenge in commercializing this solar cell technology. Since different solvent and material engineering can tailor the material properties and power-conversion efficiency, a study on the metal oxide-based all-inorganic CsSnI3Cl3-x layers is explored herein for flexible PSCs. In different processing conditions, the microstructural and optical properties are optimized to enhance the stability and performance of metal oxide-based ecofriendly flexible PSCs. Alumina is used as an efficient scaffold layer, which engineers CsSnI3Cl3-x halide perovskite material to attain efficient charge transport and long-term stability. We hope to achieve considerably enhanced stability of high-efficiency eco-friendly flexible perovskite solar cells in near future.

YAA-0006

An comparative study of extraordinary and ordinary modes in self-focusing of higher order modes of elegant hermite cosh-Gaussian laser beams in an collisionless magnetized plasma

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Abstract. In present investigation, Three-dimensional cosh-Gaussian laser beam is introduced. The self-focusing and defocusing of elegant hermite cosh-Gaussian laser beam in collision less magnetized plasma have been investigated theoretically. The final Differential equation for the beam width parameter is derived by following Wentzel-Kramers-Brillouin (WKB) and paraxial approximation through standard Akhmanov's parabolic wave equation. The final results of numerical computation are presented in the plot of beam width parameters ($f_1 \& f_2$) versus normalized propagation distance (ζ). In present investigation the author shows nonlinear effect due to different modes, magnetic field (B_0) and decentered parameter (b) on self-focusing and defocusing in collision less magnetized plasma. The results shows well enhancement in beam of self-focusing.

MgO and La₂O₃ based g-C₃N₄ /PPy for Supercapacitor Electrode

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Abstract. As the demand for efficient and reliable energy storage systems continues to grow, supercapacitors have emerged as promising candidates due to their rapid charge-discharge rates and extended cycle life. However, their lower energy density compared to traditional batteries remains a challenge. In this study, we investigate the electrochemical performance of two distinct composite materials, namely Magnesium Oxide/graphitic carbon nitride/Polypyrrole (MGP) and Lanthanum Oxide (La2O3)- modified Polypyrrole/graphitic carbon nitride (LGP), for their potential as supercapacitor electrodes. Both the composites were synthesized by a two step calcination process followed by in-situ polymerization reaction. The electrochemical performance of the composites were analyzed through cyclic voltammetry (CV), galvanostatic charge discharge (GCD) and electrochemical impedance spectroscopy (EIS) using three-electrode setup in 1 M H2SO4. The specific capacitance obtained for LGP and MGP composite was 1761.57 F g⁻¹ and 716 F g⁻¹ at 1 A g⁻¹ respectively. The better electrochemical properties of LGP composites could be due to the presence of more redox active sites in the composite which participate in faradic reaction during charging-discharging cycle resulting in higher value of specific capacitance.

YAA-0008

Synthesis of Ferroelectric Glass-ceramics: Evaluation of Crystallization Kinetics, Optical, Dielectric and Ferroelectric properties

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Abstract. The research activity on ferroelectric materials has rapidly increased since the discovery of ferroelectricity in perovskite barium titanate (BaTiO₃) ceramics in 1950. There are now more than 1000 oxide and non-oxide ferroelectric materials with extensive applications in the field of electronic industry. The structural anisotropy in ferroelectric crystals has led to many technological applications like in non-volatile random access memories (NVRAMs), ultrasound transducers, ceramic capacitors etc. The resulting structural anisotropy also gives rise to nonlinear optical properties like electro-optic effect and harmonic generation. In the electronics industry, mostly lead based ferroelectric materials have been used as dielectric materials for energy storage capacitors due to their ultrafast discharge speed, high temperature stability and stable frequency. However, the global issue of environmental pollution and energy crisis has led to the research and development of new green energy sources. In this regard, the design and development of lead free ferroelectric materials has attracted much attention worldwide. Also, with the advent of photonic age, transparent and optically active materials are required for optical amplification, switching, sensors etc. Hence development of multifunctional materials are needed which can perform the existing functions more efficiently. Ferroelectric glass-ceramics are one such type of materials which can fulfill the need of energy storage and optical/photonic applications. Generation of non-centrosymmetric, high dielectric constant ferroelectric crystals in a highly resistive host glass matrix through controlled crystallization by heat-treatments can obtain a pore-free, transparent, fine-grained, nano/ microstructured glass-ceramic material, which is crucial for energy storage and photonic applications.

Lead-free ferroelectric glass-ceramics containing the bismuth-layered structured (BLSF) crystal phases of BaBi₂Ta₂O₉ (BBT), BaBi₂Nb₂O₉ (BBN), CaBi₂Ta₂O₉ (CBT) have been synthesized successfully in silica glass matrix for the first time in the glass-ceramic route through the melt-quenching technique followed by ceramming heat-treatment. A comparative approach of non-isothermal crystallization kinetics was adopted through solid reaction reaction models and model free methods. This approach

elucidated the mechanism of crystallization in the base glasses and analyzed the rate of crystallization at different temperatures above the glass transition in order to find out the experimental heat-treatment schedule for controlled crystallization to synthesize these glass-ceramics, which was otherwise challenging. With this approach, transparent glass-ceramics containing the BLSF crystal phases were synthesized for the first time. These rare doped glass-ceramics exhibited enhanced photoluminescence, high refractive index (> 1.75) and improved third order non-linear optical susceptibilities compared to the base glasses. The role of nucleating agents like ZrO₂ was also studied in improving the rate of controlled crystallization and microstructure of the glass-ceramics, which reduced the dielectric losses and improved the hysteresis polarization. The dielectric constants were observed to increase from the base glass to the glass-ceramics upto 301 with increase in crystal volume fraction and reduction in grain boundaries in the microstructures. The dielectric losses also decreased following the same trend.

The future work would be mainly focused on the improvement of dielectric and ferroelectric properties of these glass-ceramics. Efforts can be taken to choose the glass matrix composition in a way such that the refractive index difference between the ferroelectric crystal phase and the matrix is minimized and the optical transparency become independent of the average crystal size. In such a way generation of microcrystals shall be possible in the glass matrix which would yield a transparent glass-ceramic having a large ferroelectric domain size facilitating proper hysteresis behavior with improved polarization effects. Larger maximum polarization can generate higher energy storage density which is necessary for capacitor applications. The piezoelectric and non-linear optical properties of the systems can also be explored in details for optoelectronic applications.

A Review on Progress in Innovations Based on Synthesis of Carbon Dot's

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Abstract. In Recent Years Carbon and carbon materials attracted many researcher due to their eye catching properties and their utilization in variety of applications. Literature survey revealed that macroscopic carbon materials have less abilities those as compared to nano scale materials due to low band gap and poor stability. In current review we have made an attempt to summarize the properties and application of one such nano scale product of carbon known as carbon dots.

A1-0002

A Facile Synthesis of CoMn₂O₄ - MoS₂ Nanocomposite via Co-Precipitation Approach Neha Kanaujiya^{a1}

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Abstract. The synergistic effect attracts measurable attention when the physical and/or chemical behavior of a composite material demonstrates noticeably improved properties in comparison to that exhibited by its forming components. This research work presents the synthesis of CoMn₂O₄-MoS₂ nanocomposite by using co-precipitation method. The synthesis of CoMn₂O₄ @MoS₂ nanocomposite involves the mixing of Mn²⁺, Co²⁺, and OH⁻ ions in a sequence, in the aqueous dispersion of MoS₂. The OH⁻ ions present in the solution get adsorb on MoS₂ nanosheets and make them negatively charged. Consequently, Mn²⁺ and Co²⁺ cations migrate towards the MoS₂ nanosheets and deposit over the MoS₂ sheets to form complex hydroxides which under proper annealing treatment (250 °C for 5 h) convert into well-crystallized CoMn₂O₄-MoS₂ nanocomposite. Further, numerous characterization tools such as X-Ray Diffractometer (XRD), X-Ray Photoelectron Spectroscopy (XPS), Brunauer-Emmett-Teller (BET) surface area analyzer, Fourier Transform Infrared Spectroscopy (FTIR), FESEM, High-Resolution Transmission Electron Microscope (HRTEM), and Thermal Gravimetric Analysis (TGA) are employed to explain the structural, morphological, elemental, and thermal properties of the asprepared CoMn₂O₄@MoS₂ nanocomposite.

Gamma Irradiation Effects on Structural, Thermal and Optical Properties of *CSR2* Silk Fibroin Films

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Abstract. In this work *Bombyx mori* silk fibroin (SF) films were prepared by solution casting method. Gamma irradiation of protein biopolymer films were carried out in dry air at room temperature using Co – 60 source, and radiation doses are in the range of 0-300 kGy. The unirradiated and irradiated films were characterized by X-ray diffractogram (XRD), thermogravimetric analysis (TGA) and ultra violet visible spectroscopy (UV-Vis). The observed interesting results have been tried to be correlated with structural, thermal and optical properties.

A1-0004

The Role of Trivalent Samarium on La₂MgTiO₆ Perovskite for Orange – Red Emission with 99.99% Colour Purity

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Abstract. Trivalent samarium ions are doped in the crystal structure of La₂MgTiO₆ prepared via combustion process. The XRD pattern identify the formation of single-phase orthorhombic structure with space group pbnm. Using UV-Visible info, the optical parameters such as the refractive index, bandgap and Urbach energy are computed to be 2.2705, 3.5745 eV and 484 meV respectively. When excited with 405 nm, the PL spectra show three prominent peaks at 564 nm, 601 nm and 647 nm due to ${}^{4}G_{5/2} \rightarrow {}^{6}H_{5/2}$, ${}^{4}G_{5/2} \rightarrow {}^{6}H_{7/2}$ and ${}^{4}G_{5/2} \rightarrow {}^{6}H_{9/2}$ transitions respectively. The optimized doping concentration is estimated 2% resulting from the nearest dipole-dipole exchange mechanism, above which concentration quenching is observed. The CIE and CIEL*a*b* diagram confirm orange-red emission with coordinates (0.5808, 0.4184) and colour purity 99.99%.

Electric Field Enhancement Near Plasmonic Nitrides And Carbides based Core@shell Nanoparticle For Sensing

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Abstract. New categories of materials are emerging in field of plasmonics to study the optical response of different nano particles. Nitrides and carbides are one of such promising material. In comparison to conventional plasmonics materials (metals), these emerging materials provide many advantages such as tunability; low intrinsic loss, bio compatibility, low work function etc, which are required properties of bio sensing devices. In present work, comparison of field enhancement factor of transition metal nitrides ZrN, HfN, TaN, TiN, WN and carbide material TaC in comparison to plasmonic metal gold and advantages of nitride plasmonics over conventional metal plasmonics is discussed.

A1-0006

A computational study on radioactive decay of nucleus equation using differential transform method

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Abstract: The differential transform method (DTM) and the multi-step differential transform method (MsDTM) are numerical methods are not familiar with us. The methods provide solutions in terms of convergent series with easily computable components. The aim of this article is to introduce the DTM and MsDTM as efficient tools to solve linear and nonlinear differential equations. We choose successive radioactive decay of nucleus by some mathematical methods. For accuracy of its variants by comparing the results with the Runge–Kutta method.

Exploring the Versatile Potential of GeS Nanoparticles: Photo-Catalysis and Infrared Sensing Applications

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Abstract: Germanium sulphide (GeS) nanoparticles were synthesized using the hydrothermal method. The synthesized GeS nanoparticles were characterized by X-ray diffraction (XRD), energy dispersive X-ray analysis (EDAX) and ultraviolet-visible spectroscopy (UV-Vis) techniques. EDAX results demonstrated the elemental composition confirming the presence of germanium and sulphur in desired stoichiometric ratio. The crystalline nature of the synthesized GeS nanoparticles with well-defined diffraction peaks was confirmed by XRD. Also, the crystallite size and lattice strain were evaluated by Debye-Scherrer method. Moreover, UV-Vis spectroscopy revealed the optical properties of GeS nanoparticles, including their absorbance and bandgap energy. Zeta potential measurement was carried out, providing the stability of dispersed GeS nanoparticles in water medium. The photo-catalytic activity of the GeS nanoparticles was evaluated and the parameters were determined. Furthermore, the promising characteristics exhibited by GeS nanoparticles have motivated an extension of their potential application beyond photo-catalysis. Specifically, their unique attributes have prompted the investigation of their viability in the realm of infrared (IR) sensing. The intrinsic properties of GeS nanoparticles, such as their tunable electronic structure and exceptional photon-absorption capabilities, render it as promising material for use in IR sensing technologies.

A1-0009

Thermodynamic and Surface Properties of Al-Au-Cu-Sn-Zn Liquid Alloy

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Abstract.In the context of the possibility of discovery of numerous new materials using the alloying technique, the theoretical investigation of Al-Au-Cu-Sn-Zn quinary liquid alloy was carried out using the thermodynamic approach. For this, the coefficient of R-K polynomials was optimized using the experimental values of the binary sub-system obtained from the literature. From these optimized coefficients, concentration dependence of excess Gibbs free energy was calculated as the function of Al content at five different sections of $x_{Cu}:x_{Au}:x_{Sn}:x_{Zn}$, namely, 1:2:3:4, 4:1:2:3, 3:4:1:2, 2:3:4:1 and 1:1:1:1 using Muggianu, Kohler and Chou models at 1773 K and abobe. Activities of the components were also assessed using thr Chou model in the specified sections. The surface concentration and surface tension of the liquid alloy was determined by using the Buttler equation. Further more, the variation of the surface tension with temperature was also studied in the aforementioned sections.

Effect of cation disorder on structural and magnetic parameters of ZnFe₂O₄ nanoparticles synthesized by honey mediated sol gel auto-combustion method

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Abstract. Nanotechnology contracts with the invention and practice of material using nanoscale dimension. Nanoscale dimension delivers nanoparticles a large surface area to volume ratio and thus very specific properties. Bulk zinc ferrite (ZnFe2O4) exhibits anti-ferromagnetism, with Néel temperature of 10K, is paramagnetic at room temperature. It exhibits normal spinel structure with Zn²⁺ has exclusive tetrahedral - A site preference, whereas Fe³⁺ ions occupy the octahedral - B site. Cationic disorder induced fractional overturn of the spinel structure, owing to partial immigration of Fe³⁺ ions from B to A site can prompt ferrimagnetism in nano zinc ferrite. Due to the large ratio of toxic chemicals and extreme environment employed in the chemical and physical production of these ferrites, green methods employing the use of bacteria, plants fungus have been adopted. Present work reports comprehensive study of the synthesis, structural and magnetic investigation of room temperature ferrimagnetism in ZnFe₂O₄ nanoparticles, prepared by sol gel auto-combustion mode and green synthesis method. Effect of conventional thermal annealing (ann. at 600°C for 3 hours) on magnetic properties is also reported. The structural and magnetic characteristics of as prepared and annealed ZnFe₂O₄ samples were determined by X-ray diffraction (XRD) and vibrating sample magnetometer (VSM). XRD confirms the formation of single-phase nano-crystalline cubic spinel structure of the samples.

A1-0011

A Novel Composite Cathode Material $La_{0.5}Sr_{0.5}Bi_{0.2}Co_{0.6}Fe_{0.2}O_{3-\delta}$ Fabrication for Intermediate Temperature Solid Oxide Fuel Cells

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Abstract. A novel cathode material $La_{0.5}Sr_{0.5}Bi_{0.2}Co_{0.6}Fe_{0.2}O_{3-\delta}$ ceramic was synthesized for intermediate temperature solid oxide fuel cells (IT-SOFCs) using a low-cost flash pyrolysis process, followed by conventional sintering. X-ray diffraction and scanning electron microscopy were used to examine the phase and microstructure of $La_{0.5}Sr_{0.5}Bi_{0.2}Co_{0.6}Fe_{0.2}O_{3-\delta}$ ceramic. The crystal structure, unit cell parameters, and bond length are estimated from the Rietveld refinement program. The XRD data suggested that the sample sintered at 700 °C showed a pure single phase with rhombohedral structure with $R\bar{3}C$ space group symmetry. The fracture surface of the sample sintered at 700 °C revealed a significant porosity and nano grain size (50-100 nm) through FESEM micrographs.

Josephson current across a Double Quantum Dot Josephson junction in T-Shape Configuration

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Abstract. By implementing the Keldysh non-equilibrium Green's function equation of motion approach, Josephson current has been examined across a T-shaped uncorrelated double quantum dot Josephson junction. The behavior of the Josephson current as a function of the main quantum dot energy level for varied interdot tunneling and different dot-lead coupling strengths is examined. With this configuration, we illustrate that the side-attached quantum dot offers an alternative route for electron transmission, which modifies the Josephson current by varying interdot tunneling. Further, we also investigate how the dot-lead coupling strengths affect the Josephson current.

A1-0013

A Comprehensive Examination of Ni@AgCl Nanoparticles – An Insight for Opto-Electronic Applications

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Abstract. In this study, chemical reduction approach was used to successfully manufacture Ni@AgCl core-shell nanoparticles with molar ratios of 1:1 and 4:1. The crystalline nature and face-centered cubic structure of these materials were confirmed by X-ray diffraction (XRD) investigation. Numerous characteristics, including crystallite size, dislocation density, lattice constants, volume of the unit cell, and lattice strain, were calculated using the Scherer formula and W-H plot. The findings showed that, in comparison to sample (B), which has a molar ratio of 4:1 sample (A) had a higher crystallite size and lower lattice strain. Both materials' spherical shapes were validated by morphological analysis using EDAX, which also revealed their chemical composition. Indicating indirect band gap values of 2.53 eV and 2.45 eV, the UV-Vis absorption spectra of samples (A) and (B) revealed strong peaks at 237 nm and 239 nm, respectively, confirming their semiconducting characteristics. For samples (A) and (B), photoluminescence examination revealed emission wavelengths at 397 nm and 398 nm, respectively, falling in the UV zone. In light of these results, the synthesized Ni@AgCl core-shell nanoparticles are attractive candidates for Opto-electronic applications.

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.

A1-0016

Unique optical response in monolayer doped graphene

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Abstract. Exploring the intricate interplay of scattering dynamics on graphene's transport properties is a cornerstone of this study. By systematically investigating scattering mechanisms, including intra/inter-band interactions, we unveil their profound impact on graphene's optical conductivity response under varying doping conditions. Employing an analytical approach, we utilize a semi-classical multiband Boltzmann equation to account for electron-electron and electron-phonon collisions. Surprisingly, we discover unconventional optical conductivity characteristics in doped monolayer graphene that deviate significantly from the universal conductivity. This unique departure is attributed to phenomenological relaxation rates, low doping and intraband scattering effects. Interestingly, these novel optical responses diminish at higher temperatures or in cases of overdoping, overridden by strong Drude behavior. Leveraging approximations around Dirac points, we derive an analytical framework for many-body interactions that aligns well with the Kubo approach. The insights gained not only deepen our understanding of graphene but also offer avenues for innovative electronic and optoelectronic applications, capitalizing on these distinctive phenomena.

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Surface Coupled Metal Nanoparticles for Improved SERS and RI sensing

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Abstract. Anisotropic/curved surfaces coupled with a layer of metal nanoparticles exhibit enhanced plasmonic properties than that of their colloidal counterparts, owing to the formation of raspberry or core-satellite type nanocomposites. Such nanocomposites with amplified optical features are the most reliable in applications like photocatalysis, SERS (surface-enhanced Raman scattering), and RI (refractive index) sensing, which demonstrates a high scattering probability with increased potential utility. In this present work, we synthesize Ag nanoparticles coupled onto silica spheres (of size 300 nm) intuitively functionalized with PVP (polyvinylpyrrolidone) through a single-step modified Stöber process. Careful galvanic replacement protocol has been attempted to form SiO2@Ag@Au nanocomposites, as unequivocally confirmed by our rigorous microscopic and spectroscopic studies in contrast with the conventionally formed hollow nanostructures in colloidal solutions. Furthermore, we fabricated the respective monolayer films through a liquid/liquid interface self-assembly technique, wherein a uniform array of these surface-coupled metal nanocomposites onto different substrates are formed with ease. Our study provides a novel route for the fabrication of diversified meta-structures based efficient SERS substrates having great prospects for applications in ultrasensitive chemical and biological sensing.

A1-0018

Analysis of High Pressure EOS on the Structural Properties of Gallium Compounds

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Abstract. In this particular research, we have undertaken theoretical projections of the bulk modulus, first pressure derivative of isothermal bulk modulus and the Grüneisen parameter (γ) for materials like GaN, GaAs, GaP and GaSb across varying compression values (V/V₀) by using three well known EOS viz. Brennan-Stacey EOS, Vinet EOS and Tait EOS. These EOSs are also been tested for the basic requirements revealed from the fundamental thermodynamics for in the limit of extreme compressions, as given by Stacey. It is found that at low compressions, the three EOSs viz Tait EOS, Vinet EOS and Brennan-Stacey EOS gives exactly the similar results for theoretical prediction of pressure, Bulk modulus and first pressure derivative of isothermal Bulk Modulus.

Synthesis, Structural and Spectroscopic Study of Nano Crystalline Cerium-Substituted Magnesium Ferrites

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Abstract. Nano ferrites, defined by the general formula AB₂O₄, where A represents a divalent transition metal ion and B is Fe, have garnered sustained interest due to their distinct structural, magnetic, and electrical properties relative to their bulk counterparts. The inherent high surface-to-volume ratio of nano-ferrites gives rise to fascinating behaviors, such as spin-glass-like structures due to disrupted exchange bonds, and the development of a surface layer with elevated anisotropy. The interaction of cations, particularly at surface and non-surface sites, facilitates super exchange interactions through oxygen ions, further influencing their properties. These nano-ferrites demonstrate multifunctional capabilities and find diverse applications spanning sensors, microwave components, magnetic recording, and more. An illustrative study focuses on cerium-substituted nanocrystalline magnesium ferrite, MgCe_xFe_{2-x}O₄ (x = 0.00, 0.02, 0.04, and 0.06), synthesized through the sol–gel auto-combustion method. This investigation reveals superparamagnetic behavior at room temperature and tunable DC resistivity with humidity, underscoring their potential in humidity sensing and catalytic activities. In this current work, we present a comprehensive analysis of the structural characteristics of the Mg₁. $_{\rm x}$ Ce_{x/2}Fe₂O₄ system (x = 0.00, 0.01, 0.02, and 0.03) synthesized using a low-temperature autocombustion technique. Notably, our analysis encompasses both as-prepared and sintered samples. Xray diffraction (XRD) analysis confirms the formation of single-phase materials with a cubic spinel structure. Interestingly, comparative XRD analysis of as-prepared and sintered samples sheds light on the evolution of the crystalline structure during sintering, revealing potential transformations and correlations with magnetic properties. The observed changes in X-ray density and porosity with varying ceria concentration provide additional insights into the impact of cerium substitution on the resultant structure. Raman spectroscopic analysis further corroborates the attainment of the spinel phase in the studied materials. Our investigation offers an in-depth understanding of the intricate interplay between cerium substitution and the resulting structural and magnetic attributes of these nano ferrites, shedding light on their potential applications.

A1-0020

Study of La Doped Zinc Ferrite and Their Application in Super Capacitors

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Abstract. With the increasing demand for clean energy, supercapacitors have garnersed significant interest as a promising energy storage technology. Their advantages, including high power density, rapid recharge capabilities, and long cycle life, make them appealing. Among various energy storage options, supercapacitors based on ferrites have captured attention. Research has predominantly centered on pseudocapacitive electrode materials like transition metal oxides (e.g. MnO₂, Co₃O₄, NiO) and conducting polymers (such as polyaniline, polypyrrole, and polythiophene). Within this category, spinel transition metal oxides (AB₂O₄) have gained prominence due to their unique electronic structures and the use of two metallic elements. Herein we have synthesized ZnFe_{2-x}La_xO₄ nanoparticles with varying the La content (x = 0, 0.01, 0.03, 0.05) through a cost-effective combustion method using citric acid as a fuel. Through X-ray diffraction analysis, it was confirmed that the synthesized ZnFe₂O₄ product possessed a cubic crystalline structure. The diffraction pattern, including planes (220), (311), (400), (511), and (400), confirmed the cubic spinel structure with the Fd-3m space group. No extra peak has been observed in the XRD spectrum indicating the pure form of the samples. Essential parameters such as lattice parameter, particle size, and X-ray density were calculated, while strain was evaluated using the Williamson-Hall method. In order to investigate the vibrational mode present in the samples, Raman experiment is performed which exhibited well-defined Raman active modes. The Raman spectra

revealed the presence of five Raman active modes (A1g + Eg + 3F2g) as anticipated in the spinel structure. Moreover, the obtained Raman spectra were found to be in good agreement with reported data.

A1-0021

Electrical Transport Study of Alkali Titanate of the Type A₄TiO₄ Where A Stands for (A=Li, Na, K)

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Abstract. Alkali titanate of the type A_4TiO_4 , where A stands for (A=Li, Na, K) have been prepared using high temperature solid state reaction technique employing carbonates of respective alkali metals and TiO_2 as starting materials. Electrical conductivity (σ) and thermoelectric power (S) of pressed pellets of A_4TiO_4 have been measured in the temperature range of 440K to the melting point of each Material. Results have been reported as $Log \, \sigma T \, Vs \, T^{-1}$ and S $Vs \, T^{-1}$ plots. It has been observed that σ jumps by a factor of $(10\text{-}10^2)$ at a particular temperature for each solid and reaches the value of the order of $(10^2 \, \text{to} \, 10^3)$ around 1100K. S values show anomaly at the same temperature for each solid, this temperature has been referred to as phase transition (T_P) of that solid. The ionic (σ_i) and electronic (σ_e) parts in total conductivity have been evaluated using time dependence study of dc electrical conductivity. It has been observed that contribution of σ_i to σ above T_P is more than (97 to 99%) for each solid, below T_P , it decreases but remains close to (92 to 96%) up to 500K. From these data it has been concluded that each of these materials exists in two phases. The phase above T_P is Superionic and below T_P is mixed conductor. In this phase one can expect the existence of Frankel defect and they are probably, the entity of electrical conduction. The enthalpy for the migration of these defects and heat of transport also been evaluated.

A1-0022

Dielectric, magnetic and magnetoelectric properties of laminated thick films of coppercobalt ferrite and lead zirconium titanate

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Abstract. The Magnetoelectric composites with thickness of 0.3mm of high piezoelectric voltage coefficient material, PbZr_{0.58}Ti_{0.42}O₃ and magnetostrictive material, Cu_{0.6}Co_{0.4}Fe₂O₄ were fabricated by Screen printing method. XRD analysis indicates the presence of inverse cubic spinel structure in the ferrite phase and tetragonal perovskite structure in the ferroelectric phase. The computed lattice parameters and crystallite sizes for both ferrite and ferroelectric phases correspond well with values reported for comparable systems. Based on space charge polarization mechanism, the dielectric constant and loss tangent with frequency are explained for laminated films $Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4$ and $PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3$. The magnetization hysteresis loop characteristics for both laminated thick films demonstrate that the loops are completely saturated and reveal the presence of an ordered magnetic structure. The DC resistivity graphs show that the resistivity of laminated film composites decreases with increasing temperature, demonstrating semiconductor behaviour in both layered composites. In a DC magnetic field range of 2000e to 4000e, the peak values of the ME coefficient in laminated thick film composites $Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4 \quad and \quad PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_3/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}O_4/PbZr_{0.58}Ti_{0.42}O_5/Cu_{0.6}Co_{0.4}Fe_2O_4/PbZr_{0.58}Ti_{0.42}$ Ti_{0.42}O₃ are 91 mV/Oecm and 83 mV/Oecm.

Investigating the Impact of Annealing Temperature on the Optical Properties of Europium Doped TiO₂

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Abstract. Titanium dioxide substituted with Europium (Eu³⁺) was synthesized using Sol Gel method with different molar ratios of Eu^{3+} (i.e. x=0, 0.2, 0.4, 0.6 mol %). This method employed Oxalic acid as a catalyst and Titanium Butoxide as the precursor, with Europium serving as the dopant. The annealing process was carried out at temperatures of 400°C and 600°C. Structural analysis was conducted utilizing X-Ray diffraction (XRD) patterns, which revealed crystalline planes corresponding to the facets of tetragonal TiO₂. The powders prepared at 400°C retained some anatase phase, whereas those prepared at 600°C exhibited a mixture of anatase and rutile phases, displaying higher crystallinity compared to the samples prepared at 400°C. FTIR spectra depicted the characteristic peak of the Ti-O bond stretching vibrations observed at 420 cm⁻¹ for all the samples prepared at 400°C and 600°C with some other vibration which shows presence of isolated Ti-OH groups on the surface. Optical analysis encompassed UV spectroscopy analysis with the study of absorbance and reflectance spectrum. The UV spectrum for powders annealed at 400°C showcased the absorption range in the UV region with very slight absorption in visible region. For the samples prepared at 600°C strong absorption in UV region only was observed. The indirect band gap was calculated using Tauc Plot which shows the value between 2.91 eV to 3.06 eV for prepared samples at 400°C and 3.03 eV to 3.018 eV for samples prepared at 600°C. Photoluminescence spectra provided insight into the emission spectra which shows strongest emission around 620 nm that corresponds to the electrical dipole transition ${}^5D_0 \rightarrow {}^7F_2$ of Eu³⁺ ions which give the red color in the luminescence signals. This study aimed to uncover the intricate property variations of Eu³⁺ doped Titanium Dioxide across diverse molar concentrations at two different temperatures.

A1-0026

Characterization and Synthesis of Nanocrystalline CoFe₂O₄ Ferrites Prepared by Sol-Gel Method with Citric Acid Variation

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Abstract. The objective of this study is to develop nanocrystalline CoFe₂O₄ for making them suitable for various applications such as sensors, recording devices, permanent magnets, solar cells, and magnetic drug delivery. The CoFe₂O₄ ferrite samples were prepared using the sol-gel method with varying amounts of citric acid. XRD characterization revealed a single-phase cubic structure, and the broad peak indicated the presence of nano-sized particles. The Debye-Scherrer formula was employed to calculate the crystallite size of the samples. Interestingly, increasing the citric acid content led to a decrease in the FWHM (full width at half maximum) broadening, as clearly observed in the XRD pattern. To examine the surface morphology, Field Emission Scanning Electron Microscopy (FE-SEM) was utilized for all samples, demonstrating their well-prepared spherical nature. Additionally, Energy Dispersive Spectroscopy (EDS) confirmed the elemental composition of the samples, indicating appropriate doping in the polycrystalline samples. The presence of different chemical bonds has been confirmed by the Fourier Transform Infrared Rays (FTIR) Spectroscopy.

Synthesis and Characterization of Nano-Crystalline Ni-Doped CoFe₂O₄ Ferrite for Biomedical Applications

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Abstract. A polycrystalline ferrite sample of Co_{0.9}Ni_{0.1}Fe₂O₄ was successfully synthesized using the sol-gel auto-combustion process. The X-ray diffraction (XRD) analysis provided confirmation of the cubic phase spinel structure of the sample. To ensure the absence of any impurity phases, Rietveld refinement was conducted. The sample's crystallite size, existing in the nano regime, was determined using the Debye-Scherer formula. Field Emission Scanning Electron Microscopy (FESEM) demonstrated the prepared sample's spherical nature, confirming its porous and agglomeration structural properties. Energy Dispersive Spectra (EDS) offered evidence of the elemental confirmation and purity of the synthesized nanoparticles. Additionally, the EDAX spectrum verified appropriate doping in the polycrystalline sample. Furthermore, the Fourier Transform Infrared Rays (FTIR) Spectrum, covering the range from 4000 cm⁻¹ to 500cm⁻¹, showcased a wide array of chemical interactions within the sample. The significance of this nano-crystalline Ni-doped CoFe₂O₄ ferrite lies in its biomedical applications, as it offers simplicity, cost-effectiveness, and reproducibility.

A1-0028

Theoretical Estimation of Melting Points and Heat Capacities of Coinage Metals Nanoparticles for Different Sizes and Shapes

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Abstract. In our previous article, we proposed an empirical relation between the melting point of nanostructured materials and that of their bulk counterpart. In this study, we introduce a method to determine the fraction of surface atoms relative to the total number of atoms within a nanoparticle. This method utilizes a distribution approach for surface and interior atoms within the unit cell of a nanomaterial crystal, and the derived fraction is linked to the size and shape of the nanomaterial. Additionally, we develop a proposition that correlates the relaxation factor with the presence of dangling bonds in surface atoms, based on the ratio of surface atoms to the total atoms. Subsequently, we estimate the melting points and the heat capacity for coinage metals (gold, silver and copper) across various nanoparticle sizes and shapes. Our findings demonstrate a favorable agreement with the experimentally measured values for these particles.

Optical Characterization of Nickel Doped Zinc Oxide Thin Films Deposited by RF/DC Sputtering Technique

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Abstract. At room temperature 30° C, pure zinc oxide (ZnO) and nickel doped ZnO thin films was prepared on ITO coated glass substrates by using RF/DC reactive co-sputtering technique. The main target of this experimental research work was to investigate the doping effect of nickel on optical properties of nickel doped ZnO thin films. The fabricated thin films were characterized by using Energy-Dispersive Analysis X-ray, X-Ray Diffractometer (XRD), Atomic Force Microscope, Fourier Transform Infrared Spectroscopy (FT-IR), Field Emission Scanning Electron Microscope (FESEM) and UV-VIS Spectrophotometer to investigate the doping growth, structural crystallinity, surface morphology, chemical bonding information, film thickness and optical properties respectively. The XRD information of all fabricated thin films reveals that the highly intensive peak has been found near glancing angle at 34.48° corresponds to miller indices (002), which confirmed the wurtzite hexagonal crystallite structure of ZnO that matched with JCPDS card no 36-1451. It is found that with the increasing of atomic % of nickel from 0 to 6.5 in ZnO the Crystallite size of deposited thin films increased from 8 nm to 15 nm respectively. It is also found that with the increasing of atomic % of nickel from 0 to 6.5 in ZnO the optical band gap energy of the deposited thin films decreases from 3.17 eV to 2.23 eV. Urbach energy of the deposited thin films increases from 118 meV to 243 meV with the increasing of atomic % of nickel from 0 to 6.5.

A1-0030

Extraction of Mono to Few Layers of Graphene through Micromechanical Exfoliation of Bulk Graphite

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Abstract. Graphite is an allotrope of carbon that occurs naturally. The structure is comprised of multiple layers of carbon atoms that are organized in a hexagonal lattice and are interconnected by relatively weak van der Waals forces. Graphite exhibits favorable electrical conductivity characteristics, demonstrating enhanced efficiency in conducting electricity along its layers as opposed to that perpendicular to the layers. This restriction influences the efficiency of the device within certain electrical and electronic applications. To address these challenges, a range of exfoliation techniques have been employed to achieve the production of graphene with a limited number of layers, typically ranging from single to a few layers. In this study, a straightforward and cost-effective method known as Scotch-Tape Microexfoliation was employed to produce graphene successfully. Optical images were captured to document various iterations of exfoliation. Notably, an increase in the number of iterations yielded a corresponding increase in film transparency, indicating the formation of a monolayer of graphene. Furthermore, the presence of defects in graphene was identified through the observation of the peak corresponding to the D-band in Raman spectroscopy.

Alignment of SWCNTs through Dielectrophoresis Method: A Potential FET Device

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Abstract. The process of single-walled carbon nanotube (SWCNT) formation involves the rolling of a graphene sheet into a cylindrical configuration. The present work provides the construction of single-walled carbon nanotube field-effect transistors (SWCNTFETs) on a silicon oxide (SiO2) wafer using the dielectrophoresis (DEP) technique. In the process of fabricating SWCNTFETs using DEP, semiconducting SWCNTs were incorporated in the role of the active channel component. The length of the channel was measured to be somewhere within a range of 5 µm. The fabrication of the source and drain electrodes involved the use of a 100 nm thick layer of gold (Au) through the implementation of the sputtering technique. The current-voltage (IV) characteristics exhibit a nearly ohmic contact behavior. The utilization of DEP for mounting CNTs is a straightforward and efficient method. Moreover, the manufacturing procedures involved in DEP-based device production are compatible with silicon (Si) technology processes, thereby enabling the potential for large-scale manufacturing of CNT electronic equipment on wafers. Furthermore, the device that was manufactured showed promise for use in a variety of areas, including biosensing, health management, the environment, wearable electronics, etc.

A1-0032

Synthesis of MoS₂ Nanomaterial by Liquid Exfoliation and Ball Milling: A Comparative Study

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Abstract. Industrial applications and fundamental scientific research involving the scalable development of high-quality Molybdenum disulfide (MoS₂) nanosheets continue to present significant challenges. MoS₂ is a material with a two-dimensional (2D) structure consisting of a single layer of molybdenum atoms positioned between two layers of sulfur atoms. The primary type of bonding present within each layer is primarily covalent in nature, characterized by the formation of robust chemical bonds between the atoms of molybdenum and sulfur. Nevertheless, the predominant driving force behind the interactions among the layers of MoS₂ is attributed to van der Waals forces. This study utilizes a top-down approach to synthesize MoS₂ nanomaterials from their bulk counterpart. This is achieved through the implementation of grinding via liquid exfoliation and ball milling methods. These methods effectively mitigate the influence of weak van der Waals forces that exist between the layers of MoS₂, resulting in the production of nanomaterials derived from their bulk counterparts. This study compared the above methods using Field Emission Scanning Electron Microscopy (FESEM) and X-ray Diffraction (XRD).

Morphological Analysis of MoS₂-Alumina Nanocomposite Tapes/Films: Effects of Additives and Processing Conditions

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Abstract. The sol-gel methodology has been extensively utilized in the production of metal oxide solutions, commonly known as sols. This technique represents a cost-effective and facile approach to the production of metal oxide solutions, achieved through the utilization of lower temperatures. Here, this paper presents a cost-effective and straightforward method, referred to as 'gel-cast,' for fabricating tape/film composed of a composite material consisting of alumina (Al₂O₃) and molybdenum disulfide (MoS₂). The composite material was synthesized through the even distribution of MoS₂ powder within an alumina sol, which was developed using the sol-gel method. The morphological investigations were undertaken to ascertain the characteristics of the tape/film subsequent to the introduction of additives. The composition of the tape/film was also examined both prior to and following the annealing process.

A1-0034

Optical Properties of Multiferroics BifeO₃ Nanoparticles by Sol Gel Method

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Abstract. Single Phase challenging and optical properties of BiFeO3 nanoparticles synthesized by sol gel technique to suppressing the leakage current and in improving the ferroelectricity in BiFeO3. Prepared BiFeO3 nanoparticles have been characterized to study structural, optical properties by XRD, FESEM and FTIR spectroscopy. BiFeO3 is the most interesting material which exhibits multiferroics response. BiFeO3 reveals simultaneously spontaneous properties of ferroelectric and ferromagnetic in the Single phase sample at room temperature. The multifuctionality of BiFeO3 proposes analyzing the fundamental physics as well as in many ranges of applications like in information storage, spintronics and sensors. BiFeO3 nanoparticles are synthesized by following sol gel method. Field emission electron microscopy (FESEM) images show the surface morphology of the sample and also are used to calculate the average particle size. All types of functional groups of the sample BiFeO3 as well as optical band gap are observed by the Fourier transform infrared spectroscopy (FTIR) spectra. The optical band gap of bismuth ferrite about (~2.2 eV) lies in visible range so it is applicable as photo catalyst for water splitting and degradation of organic pollutants materials.

Synthesis and Magnetic Properties of Polyhedral Fe₃O₄ Nanocrystals

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Abstract. Nanoparticles of Fe3O4 were synthesized employing a wet chemical procedure, succeeded by compacting into pellets. Diverse particle dimensions were achieved via vacuum sintering of pellets at 800°C, with durations of 4 hours and 24 hours respectively. The exploration encompassed a thorough analysis of the magnetic attributes through temperature, field, and time-dependent magnetization measurements. Measurements were executed within the temperature span of 20K < T < 300K and magnetic fields up to 7.5 kOe. Accompanying this, relaxation measurements were performed. Structural aspects of polyhedral Fe3O4 particles were scrutinized via X-ray Diffraction (XRD) patterns, with determination of crystallite size and microstrain carried out using the Williamson–Hall technique. Furthermore, in-situ chemical analysis was facilitated through an energy-dispersive X-ray (EDS). Magnetization assessments were undertaken, exploring the magnetic effect of the samples concerning temperature and field variables. Notably, both samples exhibited a ferrimagnetic state at 300K, evident from their M – T curves. This comprehensive study illuminates the magnetic attributes of nanosized Fe3O4 particles, providing valuable insights into their versatile behavior across varying conditions and augmenting the comprehension of their potential applications.

A1-0037

Tin sulfide nanoparticles as a p-type semiconductor material: synthesis and characterization Mohd Zubair Ansari^{1a} and Raunak Sharma¹

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Abstract. Researchers are looking into tin sulfide as a potential solar light-collecting material for thinfilm photovoltaic cells because it is cheap, widely available on Earth, and safe for the environment. Photodetectors, anode materials for lithium-ion batteries, thermoelectrics, and photocatalysis are potential applications of SnS in other fields. In the context of solar energy conversion, SnS has an optical band gap of 1.07 eV, an efficient absorption onset of approximately 1.4-1.5 eV, and a high absorption coefficient ($\alpha > 10^4$ cm⁻¹). The creation of Sn vacancies, which serve as shallow acceptors, causes the material SnS2 to exhibit inherent p-type doping. The fabrication and characterization of SnS nanoparticles are described in the present study. It has been demonstrated feasible to create transparent conductive SnS using an inexpensive, straightforward chemical bath deposition procedure with varying pH value (7, 8, 9, and 10). XRD, FTIR, and UV-visible have all been used to ascertain the structural and optical characteristics of SnS nanoparticles in the present investigation. The objective of this study is to examine the impact of various pH levels on the developed tin sulfide (SnS) nanoparticles. The Xray diffraction pattern reveals information regarding the structural analysis and crystallite size of SnS nanoparticles, with a notable trend of decreasing size observed as the pH value increases. The crystallite sizes corresponding to pH values of 7, 8, 9, and 10 are 30.54 nm, 19.67 nm, 10.15 nm, and 05.38 nm, respectively. The estimation of the optical bandgap energies of the SnS nanoparticles was conducted by using the use of a Tauc plot. The obtained values were 2.27 eV, 2.35 eV, 2.43 eV, and 2.47 eV, in sequential order. The decrease in SnS nanoparticle crystallite size was noticed as the pH values increased from pH 7 to pH 10. The observed phenomenon of the band gap energy of SnS nanoparticles increasing as the crystallite sizes decrease can be attributed to the quantum confinement effect. The FTIR spectra provide validation of the dominant bond stretching involving sulfur (S) and tin (Sn) atoms. The utilization of SnS nanoparticles as an absorber layer in SnS-based heterojunction solar cells becomes viable upon obtaining improved optical characteristics in the nanoparticles.

Comparative Study of Radiation Shielding Parameters for NiFe₂O₄ And CoFe₂O₄ Nanoparticles.

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Abstract. In this present work Sol-gel auto combustion technique was used for the preparation of NiFe₂O₄ and CoFe₂O₄ ferrite samples and the investigation of their gamma ray shielding characteristics experimentally. Gamma ray shielding parameters are determined with different gamma ray sources and NaI(Tl) scintillation detector and theoretically via Phy-X /PSD Software program. The comparative study of the linear attenuation coefficient(μ), mass attenuation coefficient (μ / ρ), Half and Tenth value layers (HVL, TVL), Mean free path (MFP), for manufactured spinel ferrites is carried out using Phy-X /PSD Software program at 122–1330 keV. The experimental results revealed good agreement with the theoretical values. The proposed nanoparticles are well established to be useful for the development of improved γ -radiation shielding.

A1-0039

Structural, Morphological, and Spectroscopic Insights into Nanocrystalline Mn-Doped ZnFe₂O₄ Ferrite for Technological Applications

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Abstract. The sol-gel method was employed to synthesize nanocrystalline Zn_{1-x}Mn_xFe₂O₄ ferrite samples, with x values of 0.2, 0.4, 0.6, and 0.8. Characterization of these samples was conducted using X-ray diffraction (XRD). The results of Rietveld refinement clearly indicated a single-phase cubic structure. The presence of nanoparticles was evident from the broad peak, and the Debye-Scherrer formula was applied to compute the crystallite size, confirming the nano-scale nature of the prepared samples. The XRD pattern (Figure 1) highlighted that changes in pH influenced the full width at half maximum (FWHM) broadening. Notably, an increase in citric acid content led to a reduction in FWHM, as observed in the XRD pattern. Field Emission Scanning Electron Microscopy (FESEM) was employed for surface morphological analysis across all samples, revealing their well-prepared spherical nature. Elemental confirmation was achieved through Energy Dispersive X-ray Spectroscopy (EDAX), which verified appropriate doping in the polycrystalline samples. The Raman spectra provided insights into the vibrational modes present in the samples. Fourier Transform Infrared Rays (FTIR) Spectroscopy confirmed the presence of distinct chemical bonds. The significance of ZnFe₂O₄ ferrites lies in their diverse biomedical and technological applications, including biosensors, magnetic separation, targeted drug delivery, magnetic resonance imaging (MRI), and magnetic hyperthermia.

Ultrafast Flash Synthesis of Vertically Oriented Exfoliated Reduced Graphene Oxide Decorated with Uniformly Dispersed Ultra-Small Metal Nanoclusters as Superefficient Catalyst for Hydrogen Evolution Reaction

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Abstract. The electrocatalytic hydrogen evolution reaction (HER) facilitates the conversion of renewable energy sources, such as solar or wind power, into chemical energy by efficiently producing green hydrogen (H₂) fuel through water splitting. Currently, state-of-the-art electrocatalysts predominantly rely on precious metals like Pt, Ru, Ir, and, Pd due to their exceptional efficiency and long-term stability. However, the limited availability and high costs of these noble metals raise concerns about the economic feasibility of electrocatalytic green hydrogen production. The primary challenge in developing sustainable HER lies in readily available substitutes for noble metals or reducing the amount of usage of noble metals in electrocatalysts without compromising their efficiency. The efficiency could drastically be improved and the amount of usage could simultaneously be reduced by reducing the size of the metal catalysts from bulk to uniformly dispersed nanoclusters (1 nm-2 nm) or even single atoms. Controlled uniform atomic dispersion of tiny metal nanoclusters (M-NCs) over a highly conducting support (e.g., graphene) is crucial for efficient and low-cost electrocatalytic HER. To address all the challenges, here we are reporting a novel ultrafast flash Joule heating technique introduced by James M. Tour and his co-workers, for nano-dispersion of ultrasmall M-NCs over vertically oriented exfoliated reduced graphene oxide (VErGO) firmly anchored to commercial carbon cloth (CC) (M-NC@VErGO@CC, M referred to Pt, Ru, Ir, Pd, Ni, Co, Fe, V, etc.,). This novel strategy is a facile twostage process for the synthesis of M-NC@VErGO@CC (Fig. 1 (a)). In the first stage, the CC was dipcoated with graphene oxide (GO) and metal salt (MS) solution (GOMS@CC) and in the second stage, the facile ultrafast flash heating (Joule heating by an ultrashort current pulse (50 ms)) helps reducing and exfoliating the GO into VErGO and simultaneously dispersing the metal salt into ultrasmall M-NCs over VErGO within just 50 milliseconds (Fig. 1 (b)). The synergy between highly conducting VErGO and uniformly dispersed M-NCs gives rise to high activity with ultralow overpotentials for HER. The unique flash heating technique is efficient in terms of time and energy cost, and its ability to simultaneously control the reduction-cum-exfoliation of GO and size of nanoclusters (single-atom to ultrasmall (1 nm - 2 nm) NCs) to develop super-efficient HER catalysts M-NC@VErGO@CC.

A1-0041

Study of The Structural, Morphological and Optical Properties of Natural Thin Layer (Nanoparticles) Deposited on Rocks

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² Department of Chemistry, Faculty of Applied Science, Taiz University, Taiz 6803, Yemen; *sameerahalqadasy@gmail.com (Sameerah S.S. Alqadasy); chishtysq@gmail.com (S. Q. Chishty). hakimalariqe@yahoo.com (Hakim Q. N. Al-arique); wadahm2007@yahoo.com (W.M. Al- Asbahy). Abstract. In truth, nanotechnology may be very well sourced from nature. It offers us a variety of tiny particles, including mineral particles found in the air, on the surface of rocks, and inorganic ash and soot. Rock samples collected from (Hanuman Tekdi Parvati nagar) region, Aurangabad they were analysed by using X-ray diffraction (XRD) spectroscopy to determine mineral composition, FT–IR spectra showed absorption peaks of different functional groups, FE–SEM images revealed the morphological of samples particles and the bandgap energy (Eg) of the nanoparticles determined by UV–VIS spectrophotometry. The XRD spectroscopy results indicate that the samples were polycrystalline nature and contain varies of minerals from one sample to another, sample (a) contains (Cu,Si,Zn,Ca) and sample (b) have minerals (Fe,Ti,Sn,Ni) in addition to metals ,FT–IR spectra showed absorption peaks of different functional groups (C=C, O-H, C-H, Si-O-Si, Zn-O,...ect), FE-SEM images shows aggregated nanoparticles with different surface morphologies in terms of size and form and the bandgap energy (Eg) for sample (a) and (b) were 4.30 and 3.75 ev respectively.

Role of ZnO-MoO3 Nanocomposite As Photocatalyst

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Abstract Nanocomposite materials have garnered significant interest due to their properties arising from the combination of distinct components. The present work focuses on the synthesis, characterization, and photocatalyst application of ZnO-MoO3 nanocomposites. The individual properties of zinc oxide (ZnO) and molybdenum trioxide (MoO3) make them promising candidates for photocatalytic applications, and their integration at the nanoscale offers the potential for enhanced performance. The doping of MoO3 and ZnO was effectively carried out by a simple precipitation method with a sonication technique. The phase study and surface morphology of MoO3-ZnO nanomaterial were characterized by means of X-ray diffractometer and FE-SEM analysis. The photocatalytic activity was established by testing the degradation and decolorization of RhB dye from an aqueous solution with sunlight under primary analysis initial concentration of dye, stability and reusability.

A1-0043

Synthesis of Cr-Doped Titanium Dioxide Nano-particles through Microwave to Enhance the Structural & Optical Properties

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Abstract. Metal doping in metal oxides enhances the optical activity of material. Therefore Cr-doped TiO2 nanoparticles using Chromium oxide and titanium butaoxide have been prepared. In the present study, the synthesis and characterization of Cr-doped TiO2 through microwave is reported. The resulting lemon green colour material was obtained. This Cr-doped TiO2 characterized by x-ray diffraction (XRD), FTIR spectrometer and UV-Visible spectroscopy. The XRD pattern reveals the presence of TiO2 & Cr peak and the shifting of an absorption edge towards the visible region has been observed in UV- visible spectra. The band gap of the Cr-doped TiO2 was found to be decreased as compare to anatase TiO2. This band gap lowering enhances the absorption of sunlight giving rise to improved power conversion efficiency.

Investigation of MWNT-enabled anode for Energy Storage Applications

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Abstract. The detrimental effects of climate change and global warming have become major concerns due to an increase in carbon footprints across the globe. One of the techniques to minimize carbon emissions is the use of clean & green energy while limiting the use of fossil fuels. Interestingly, rechargeable batteries based on lithium-ion technology serve the purpose due to their stability and reliability. Specially, lithium-ion batteries have gained more attention due to their higher energy density, high coulombic efficiency, high discharge power and longer cycle life. Graphite is still employed as an anode material because of its simple and highly ordered carbon structure. However, the search for new materials and their hybrids cannot be ignored as graphite's interaction with electrolytes lead to poor performance on prolonged usage. MWNTs (Multi Wall Nano Tubes) exhibit exceptional electrical conductivity, a large surface area, and mechanical strength, contributing to an enhanced lithium storage capacity and rate capability, ultimately leading to improved battery performance. Additionally, we have investigated the material using various characterization techniques to ensure that the materials have been synthesized in the correct phase and purity.

A1-0045

Synthesize of low-cost carbon soot material and their structural investigation Shivani Dhall¹ and Kapil Sood²

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Abstract. In the present work, we have reported simple and cost-effective route for the synthesis of candle carbon soot (CCS) layer at room temperature using candle flame. The main objective of this work is to optimized the layer of CCS and control on their graphitic order by sintering in different temperature conditions. We have found that sintered process effectively changes their structural properties as clearly indicated by XRD and Raman spectra. The mechanism of CCS self-assembly is explained with their structural and morphology properties. The controlled on CCS films have the potential application in gas sensor, photocatalysis, solar cells and lithium-ion batteries.

Synthesis of Zn_{1-x} Ni_x O: (x=0, 0.07) nanoparticles using Ananas Comosus leaves extract and their energy storage application

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Abstract. Green synthesis is a simple, time and cost effective method in which plant extract is used as a stabilized and size-reducing agent during the process. This paper reported synthesis of nickel doped and an undoped zinc oxide nanoparticle uses ananas comosus leaves extract as capping agent. The synthesized samples were characterized by UV-Vis, XRD and SEM-EDX for finding scope in energy storage sector. The study reported that optical band gap of doped samples was shrunk 8.6 % with respect to pure, which reflected some position occupied by Nickel element in the unit cell and may be the one of reasons that number of free electrons increased due to High atomic number and also confirmed by results of absorbance spectra. The XRD pattern confirmed hexagonal wurtzite structure and lattice index changed in one direction. Most intense diffraction peaks observed in (1 0 1) plane and calculated Debye-Scherer average particle size varies 46.34 to 43.77 nm. Surface analysis by SEM-EDX techniques confirmed the purity of the samples and calculated irregular nano size shaped varies between 21-60 nm.

A1-0047

Effect of strontium doping on Thermal Stability, Electrical Susceptibility, and AC Conductivity of Gel Grown Sr_{0.0127} [Ni_{0.1953}: Cd_{0.7919} C₂O₄]. 3H₂O Crystals

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Abstract. New crystals of strontium doped nickel cadmium oxalate (SNCO) trihydrate were grown by single diffusion method in silica hydro gel by optimizing various growth parameters. The existence of Sr, Ni, Cd, C and O elements in the crystal lattice were identified using energy dispersive X-ray (EDX) analysis. The occurrences of C-O, C=O, C-C, O-H and M-O bonds were observed using Fourier transform infrared (FTIR) spectrophotometer. Thermal studies (TG/DTG/DTA/DSC) show the high thermal stability (Ts>600° C) of grown crystals. The high energy gap (Eg=5.4207 eV) from the UV-Visible absorption spectroscopy confirms the insulating behavior of the crystals. Existence of high electrical susceptibility, χ_e =2.62 shows the defect less crystalline nature. Low electrical conductivity, σ_{DC} = 0.77×10⁻⁶ S.m⁻¹, high leakage resistance (51.89M Ω) and the variation of dielectric constant, dielectric loss, AC conductivity (10⁻⁵ to 10⁻⁴ S.m⁻¹) with frequency were studied and reported.

Scaled Factorial Moment Correlation Study in Pb+Pb Collisions

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Abstract. The essence of experimental ultra-relativistic heavy ion collision physics is the production and study of strongly interacting matter at extreme energy densities, temperatures and consequent search for equation of state of nuclear matter. For the present analysis, data from the Photon Multiplicity Detector (PMD) is used. The focus of the analysis has been to examine pseudo-rapidity distributions and intermittent behaviour in terms of moment of event factorial moment obtained for the γ -like particles in pre-shower Photon multiplicity detector. We also attempt to model the fluctuations seen in the data using a simple multi-source model. This allows the extension of scaled factorial moment analysis to bin sizes smaller than those accessible to other experimental techniques.

A1-0049

Bismuth Sulphide Nanoparticles: Synthesis, Characterization and Pressure Sensing Application N. T. Sailor^{1, b)}, N. N. Prajapati¹, H. M. Patel², S.P.Sikligar¹, P. B. Patel², H. N. Desai², J. M.

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Abstract. The unique properties and potential applications of Bismuth Sulphide (Bi_2S_3) nanoparticles have attracted great attention in various applications. Bi_2S_3 is classified as a V-VI semiconductor group, belongs to the main group metal chalcogenides of $A^V_2B^{VI}_3$ ($A=Bi;\ B=S$) type. The hydrothermal technique is utilized for synthesizing these nanoparticles. The structural properties of the synthesized Bi_2S_3 nanoparticles are determined through X-ray diffraction (XRD). The Williamson-Hall model is used to evaluate parameters: grain size and lattice strain. Compositional analysis is carried out using Energy Dispersive X-ray analysis (EDAX). The thermal activation energy of the nano particles are calculated through thermo-gravimetric analysis (TGA). With the aid of polyvinyl alcohol (PVA) based solution, synthesized Bi_2S_3 nanoparticles are used to formulate pressure sensor and its responsitivity is detected over a pressure range from 5.8 kPa to 25.5 kPa.

Metal Ion Doped Hydroxyapatite

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Abstract. Hydroxyapatite [Ca₁₀(PO₄)₆(OH)₂] is a calcium phosphate mineral used as a coating for orthopedic body implants, teeth & bone filling material shows excellent bioactivity & biocompatibility but lacks in Photocatalytic & antibacterial properties, which can be improved by replacing calcium ions with metal ion doping such as silver, zinc, and strontium, copper, magnesium etc. provides excellent photocatalytic, antibacterial, mechanical & electrical properties. Metal ion doped hydroxyapatite [Ca_{10-x}M_x(PO₄)₆(OH)₂] can be synthesized by various methods such as wet precipitation method, Hydrothermal method, microwave method & many more. Among these wet precipitation method is most beneficial due to a few advantages like simple, easy & moderate synthesis temperature provide good crystallites. hence investigators must be familiar with Research & investigations carried out in the relevant research area. Hence the present study is intended to explore the various aspects of different metal ion doped hydroxyapatite for the good quality Biomaterial also providing good photocatalytic activity & Antibacterial properties. Finally, some conclusions drawn from the study for future research scope which will be helpful to a new researcher in the field of metal Ion doped hydroxyapatite.

A1-0051

Effect of Precursor Concentration on Various Properties of Cadmium Oxide Nanoparticles

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Abstract. Cadmium Oxide nanoparticles (CdO NPs) were successfully synthesized using chemical coprecipitation method by varying the concentration of precursor solution (CdCl₂.H₂O). Further, the morphology and chemical composition were investigated using Field Emission Scanning Electron Microscope (FESEM) and Energy Dispersive X- Ray (EDX) analysis respectively. The Fourier Transform Infrared Spectrum reveals the Cd-O bonding and presence of other functional groups. The crystalline behavior, crystallite size and miller indices were analysed using the Powder X-ray Diffraction (PXRD) method. The energy gap in the range of 2.32 eV to 2.95 eV was obtained from the UV-Vis spectral studies. The conductivity measurements confirmed the semiconducting nature of the grown CdO NPs.

Nanorods preparation with nanoporous membranes

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Abstract. The transport using nanopores single/multi-nanopores membranes offers many technological applications. In order for the membrane to be applied in membrane technology, it is necessary to make membrane from foils according to their use. In addition, the fabrication of nanopores in membranes must be economical, durable and scalable. Nanoporous membranes cover a wide range of materials such as inorganic (metals, ceramics etc.), organic (polymeric), or composite materials. The pore size is controllable as it depends on the nature of energetic incident ions, target materials, etching conditions, etc. In this study, nanorods prepration studies of cylindrical nanopores of polymeric track etched membrane have been carried out. In addition, the fabrication of nanorods in membranes is economical and scalable.

A1-0053

Synthesis of Large Area Graphene Using Thermal CVD

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Abstract. Graphene, two-dimensional allotrope of Carbon, has gained tremendous attention due to its exotic mechanical and electronic properties. Chemical vapor deposition (CVD) of graphene on copper foils has become a key technique for the preparation of high-quality, large-area graphene sheets for use in practical applications. Present study covers the growth of large area multilayer graphene on copper foil substrate. Scanning tunneling microscopy (STM) confirms the honeycomb structure of the graphene. Surface morphology of the grown layer is characterized using Field emission scanning electron microscopy (FESEM), which confirms the synthesis of multilayer graphene on copper foil with domain size greater than 225 μ m. To investigate the chemical bonding and valence state in the structure, X-Ray photoelectron Spectroscopy (XPS) has been employed, which confirms the sp^2 bonding between the carbon atoms. The three peaks at 284.8 eV, 285.7 eV and 288.35 eV are attributed to the sp^2 carbon bonds, sp^3 carbon bonds and O - C = O bonds, respectively. Raman spectroscopy counts the layers by comparing the peak intensities of the G and 2D bands.

Formation of Nano -Microstructures in LC Media via Self-assembly of Silver Quantum Dots for Plasmonic Studies

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Abstract. Metallic nanoparticles dispersed within liquid crystal (LC) matrices have garnered significant attention due to its potential for tailoring tuneable optical and electronic properties in self-assembled silver dots. The unique combination of plasmonic nanoparticles and 6CHBT LCs offers a versatile platform for manipulating light-matter interactions at the nanoscale. Over the past few decades, quantum dots-based semiconductor industries have progressed rapidly, and a variety of mediums have been used to synthesize silver nanoparticles (NPs) and its hierarchical nanostructures. Ag-based QDs are semiconducting nanomaterials and have drawn interest for a variety of applications, including antibacterial, photocatalyst, imaging, detection and sensing. The dispersion of Ag QDs within LCs can lead to substantial modifications in the material's optical and electro-optical properties. The formation of self-assembled structures of the silver nanoparticles is confirmed by the FESEM and optical microscope images. Optical Microscope and FESEM images of Silver doped 6CHBT shows that nanomicro spheres and silver-dots one dimensional array like morphologies are formed. We have used HRXRD, FTIR, Raman, UV-vis-nir data to explore it.

A1-0055

Investigations on the Effect of various Fuels on the Synthesis of Strontium Oxide Nanoparticles

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Abstract. The Solution combustion method has been employed in the synthesis of various nanomaterials due to its advantages like low operating temperature, less time consumption, and high yield of nanoparticles. In the present work, solution combustion synthesis has been used to synthesize strontium oxide (SrO2) nanoparticles using strontium nitrate (Sr(NO3)2) as an oxidizer. In order to study the effects of different fuels on the synthesis of SrO₂ nanoparticles, different fuels like urea (CH4N₂O), citric acid (C6H8O7) and glycine (C2H5NO2) were used. The synthesized nanoparticles were subjected to various characterization techniques such as X-Ray Diffraction (XRD), Fourier Transform Infrared (FTIR) spectroscopy and UV Visible (UV-Vis) spectroscopy for analyzing the structural and optical properties of synthesized samples. The XRD result confirms that the samples are crystalline in nature and the crystallite sizes were found to be 49.59 nm, 49.33 nm and 48.47nm for urea, glycine and citric acid based SrO2respectively. The FTIR results shows that there is bending and stretching of bonds because of H-O-H, -OH, and C=O groups. The bandgap (Eg) of the synthesized samples was calculated using UV-Visible spectra and are found to be 5.08 eV, 5.83 eV and 5.72 eV for SrO2 synthesized using urea, glycine and citric acid respectively. The results shows that the SrO2 using CH4N2O has less bandgap and SrO₂ synthesized using C₂H₅NO₂ has less crystallite size. The results will be discussed in details at the conference.

Modification of the properties of α-Bi₂O₃ nanoparticles using ⁶⁰Co gamma radiation

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Abstract. The area of nanoscience and nanotechnology has seen a tremendous growth in the past few decades because of the unique and enhanced properties of the nanomaterials compared to their bulk structures. There have been numerous studies to alter the properties of nanostructures among the research community to harness the full potential of materials at nanoscale. Therefore, in the present study, efforts have been made towards changing the properties of the monoclinic bismuth oxide (α-Bi2O3) nanoparticles by irradiating them with 60Co gamma radiation. In this work, a simple solution combustion route was adopted to synthesize α-Bi₂O₃ nanoparticles using bismuth nitrate [Bi (NO₃). 6H2O] and citric acid [C6H8O7] as oxidizer and fuel respectively. In order to study the effect of irradiation, the precursor solution and also the nanoparticles of Bi₂O₃ have been irradiated with 25 kGy gamma radiation. The obtained unirradiated pristine α-Bi₂O₃, precursor solution and nanoparticle irradiated samples were characterized using various techniques to study their properties. X-ray Diffraction (XRD) was carried to study the structural properties and Fourier Transform Infrared Spectroscopy (FTIR) was carried out to study the optical characteristics of the synthesized samples before and after irradiation. The XRD patterns are shown in figure 1 and the crystallite size calculated was found to increase with the irradiation compared to unirradiated sample which can be attributed to the increase in crystallinity of the sample by the creation of defects due to ionization with high energy ⁶⁰Co gamma radiation. The FTIR spectra is shown in figure 2 and reveals the stretching vibrations of the bonds present in the sample. It can be observed that there are minimal changes in the intensity and the positions of the bonds with irradiation indicating the stability of the monoclinic phase of Bi₂O₃.

A1-0057

Gamma Ray Shielding Properties Of Mg, Ni, Zn Spinel Nano Ferrites S. N. Kane^{1, a)} and R. Verma^{1, b)}

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Abstract. Owing to extensive usage of radioactive materials in today's world, it is essential to use them with enough care, safely. Lead, Concrete are commonly used as radiation-shielding materials. Lead causes serious health problems including high blood pressure, damage to the brain, nervous system, hearing and speech problems etc., whereas concrete has number of drawbacks including prolonged use induced cracks, reduction of structural strength, density due to the presence of water. So, alternative radiation shielding materials need to be developed that are corrosion resistant, biocompatible, capable of being shaped into slim, compact designs with excellent structural integrity, endurance and exhibiting improved radiation protection properties. Therefore, in the present work, we explore the potential application of following spinel dry gel samples: Ni-ferrite (labelled as NF, x-ray density = 5.37 g/cc, grain diameter = 30.7 nm, lattice parameter = 0.8337 nm); Zn-ferrite (labelled as ZF, x-ray density = 5.33 g/cc, grain diameter = 27.6 nm, lattice parameter = 0.8437 nm); Mg-ferrite (labelled as MF, x-ray density = 4.52 g/cc, grain diameter = 28.8 nm, lattice parameter = 0.8377 nm) as gamma-radiation shielding materials. Radiation shielding properties: linear attenuation coefficient (LAC), mass attenuation coefficient (MAC), half value layer (HVL), tenth value layer (TVL), mean free path (MFP), effective atomic number $(Z_{eff.})$, effective electron density $(N_{eff.})$, effective conductivity $(C_{eff.})$, energy absorption, exposure buildup factors (EABF, EBF) in the photon energy range 0.008 - 15 MeV are computed by Phys-X / PSD software [1]. Figure 1(a - d) respectively gives the energy dependence of MAC, LAC, HVL, TVL for studied NF, MF, ZF samples. Obtained results reveal strong compositional dependence of shielding parameters: LAC, MAC, HVL, TVL. EBF, EABF increase with increasing MFP (between 1-23 cm), shows strong compositional dependence. Present results suggest potential use of spinel nano-ferrites (MF, NF, ZF) in radiation shielding and/ or protection. Detailed results will be presented.

A1-0058

Optical Analysis of MoS2 and its Hybrid Sheets

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Abstract Micromechanical exfoliation, one of the most commonly used synthesis techniques in materials, has gained prominence as a highly effective and adaptable method for exploiting two-dimensional (2D) materials, such as graphene, transition metal dichalcogenides (TMDCs), borophene, molybdenum disulfide (MoS₂), etc. The integration of MoS₂ into various applications such as electronics, optoelectronics, sensors, and energy storage devices has been driven by its exceptional properties, such as lower and tunable band gap and better adsorption effect. This work presents the use of this technique to synthesis MoS₂, graphene along with MoS₂-graphene hybrid structures on a (111) silicon wafer. Optical images gathered proved the fabrication of large-scale MoS₂ and graphene. Raman spectroscopy was employed to characterize the 2D sheets of graphene, MoS₂, and its hybrid materials. The characteristics of Raman peaks of E^1_{2g} and A_{1g} were measured at 384.22 cm⁻¹ and 409.48 cm⁻¹, respectively. The peak separation between these two peaks, i.e., the value of Δk , was found to be 25.26 cm⁻¹, proving that the multilayer 2H phase of MoS₂ was formed. This paper also comprehensively analyses the exfoliation processes' mechanisms, emphasizing the intricate relationship between van der Waals forces, interlayer bonding, and external forces. Also, it provides a succinct summary of recent studies that have concentrated on the optical characterization of MoS₂ monolayers.

A1-0059

Revealing the strain modulated quantum capacitance in BX (X= N, P, As and Sb) monolayer

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Abstract. After the discovery of 2D graphene, more research on 2D materials is taking place due to its high surface-to-volume ratio for energy storage. In this work, we have applied the biaxial strain from -10% to 10% with a difference of 2% on boron pnictides (BN, BP, BAs and BSb) monolayer and found its quantum capacitance (QC) for the application as supercapacitor electrodes. Our research reveals that owing to the BN large band gap, maximum QC is achieved 271.32 μ F/cm² at without strain (0%) and decrease during compression and tensile strain. The highest QC for BP is attained by 197.98 μ F/cm² for -10% compressive strain, and this value is 34.42% greater than the without strain quantum capacitance. For BAs and BSb, the QC value reached upto 237.50 μ F/cm² and 280.15 μ F/cm², respectively, at 10% tensile strain. This quantum capacitance is 59.60% and 108.35% higher than the without strain for BAs and BSb, respectively. We also explore the surface storage charge to specify the type of electrode for the energy storage applications.

Synthesis and Antibactarial evaluation of Novel Phenol based 1, 2, 3- Triazole by using the magnetically active Fe₃O₄.Cu₂O nanocatalyst

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Abstract. Substituted Phenol based novel 1,2,3- triazole derivatives are synthesized via click chemistry approach efficiently by using the magnetically active Fe₃O₄.Cu₂O nanocatalyst and characterized by the ¹H NMR, ¹³C NMR, Mass and IR spectroscopy. The nanocatalyst required for completion of reaction in lower concentration and recovery of nanocatalyst very easily and reusable up-to the five cycle without significant loss of catalytic properties. The catalyst was characterized by powder XRD, TEM, SEM and IR spectroscopy. For completion of the reaction required shorter time, better yield and easily available starting material with eco-friendly solvent condition. After synthesis of novel derivative are used to check out the biological activity and it observed that such derivative shows potent activity against Antibacterial stain.

A1-0062

Phytofabrication of NiO/g-C₃N₄ Nanocomposites using *A.indica* Leaf Extract for Sustainable Environmental Applications

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Abstract. Excessive water contamination has become a serious issue all over the world. Recently, green chemistry has gained lots of attention as it helps in designing safe, low-cost, and ecological photocatalysts that can help in the removal of harmful pollutants from wastewater. The present work focuses on phytoextract inspired synthesis of nickel oxide doped graphitic carbon nitride nanocomposites for photocatalytic and antibacterial activities. NiO nanoparticles were synthesized using leaf extract of the Azadirachta indica (Neem) plant, and urea derived graphitic carbon nitride was prepared using a thermal polymerization process. Here, Plant leaf extract works as a stabilizing as well as capping agent in the synthesis of NiO nanoparticles. The NiO/g-C₃N₄ nanocomposites were synthesized by varying millimolar concentrations of NiO nanoparticles (1:1, 2:1, and 3:1) and keeping the concentration of graphitic carbon nitride constant. The synthesized nanocomposites were calcined at 550°C and characterized using various analytical techniques such as UV-Vis, XRD, FTIR, PL, SEM, and EDX mapping. The prepared nanocomposite series was further examined for the photocatalytic activity of methyl orange, rhodamine B, and rose bengal dyes. Antibacterial activity against E.coli and S.aureus bacteria was also investigated for prepared nanocomposites. It is observed that the prepared nanocomposites exhibit enhanced dye degradation efficiency and excellent antibacterial activity. Owing to high photocatalytic and antibacterial efficiency along with environment friendly nature, green route synthesized NiO/g-C₃N₄ nanocomposites may be utilized for sustainable development or other potential applications such as molecular sensing, bioimaging, energy storage, organic pollutant removal, and even disease diagnosis.

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Unveiling the Structural and Morphological properties of V2O5 Nanostructures for Photocatalytic Dye Degradation

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Abstract. Vanadium Pentoxide (V_2O_5) is gaining more attention due to its specific physical, chemical and optical properties and shows its superior properties at the size range of nanoscale [1]. Among all the transition metal oxides, V_2O_5 has gained huge research interest due to its layered structure, most abundant, and cost-effectiveness [2]. In this work, co-precipitation method is used for synthesis of V_2O_5 nanostructures. The synthesized V_2O_5 nanostructure were characterized by X-ray diffraction, Raman spectroscopy, Scanning electron microscopy and energy dispersive X-ray spectroscopy (EDAX) analysis for investigation of the structural, vibrational, morphological and elemental composition of as synthesized material, respectively. X-ray diffraction analysis stands for the growth of the synthesized nanostructure is in pure orthorhombic phase. Raman analysis confirms the layered structure of V_2O_5 . The FESEM micrograph confirmed the formation of nanorods. The EDAX characterization showed the appropriate elemental compositions of vanadium and oxygen elements. Furthermore, photocatalytic activity of the samples will be investigated by using methylene blue dye degradation under a solar simulator lamp.

A1-0064

Development of cost-effective portable NH3 gas sensor based on V2O5 nanorods

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Abstract. In recent times, the increase of the concentration of toxic gases such as NO₂, CO, CO₂, NH₃, hydrocarbons and petroleum products etc. are one of the most important issues caused for environment air pollution as well as global warming. Hence, it is necessary to address the global problem to decrease the concentration of toxic gases in the environment and also the production of these gases from human related activities. One of the most promising applications of gas sensor is to monitor the air quality and the environmental air pollution. In view of gas sensing application V₂O₅ is one of the most promising candidates due to its unique physical, chemical and optical properties with layered structure, easy to synthesize material for commercial as well as industrial uses [1,2]. In this study, vanadium pentoxide (V2O₅) nanorods have been synthesized by co-precipitation method using commercial vanadium pentoxide and oxalic acid as a starting material and confirmed the nanorods like morphology by FESEM analysis. The XRD analysis stands for orthorhombic phase formation of V₂O₅ nanorods and Raman analysis confirmed the layered like structure of V₂O₅ nanorods. Whereas, the elemental composition spectra and elemental mapping were studied by EDX characterization and showed the appropriate elemental compositions of vanadium (V) and oxygen (O) elements. Further, we propose the fabrication of gas sensing device based on as synthesized V₂O₅ nanorods towards NH₃ gas sensing.

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Microstructural investigations on Hydrothermally grown Vanadium pentoxide (V₂O₅) nanomaterials

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Abstract. Vanadium Pentaoxide (V_2O_5) has got wide applications in the field of energy storage, gas sensing, energy harvesting, photocatalysis, etc. It has attractive structural, optical as well as electronic features [1]. It shows optical band gap near about 2.3 eV. We herein reported the synthesis of Vanadium pentaoxide nanomaterials using hydrothermal method. Synthesized nanomaterials was investigated structurally using Scherrer method, Williamson-Hall method. Various structural parameters such as crystallite size, dislocation density, microstrain, stress etc. has been calculated using Scherrer, and W-H plot method. These syntheses were carried out at various concentration of Vanadium source (Ammonium metavanadate NH₄VO₃). Synthesized precipitate was filtered out and dried using IR lamp. Atmospheric ambient annealing at temperature 500°C was carried out for 5 hours. Structural probing was done using X ray diffraction (XRD) technique. JCPDS (41-1426) confirms the formation of orthorhombic structure. Scherrer formula used to obtain the crystallite size, dislocation density and Crystallite size shows variation upon varying concentration of vanadium source. Williamson-Hall method was used to obtain the crystallite size, macrostrain, and stress. Three models of W-H plot were used to obtain the structural parameters. Uniform deformation model (UDM), Uniform stress deformation model (USDM), and Uniform deformation energy density model (UDEDM) were used to obtain the structural features. Further, obtained values were comparatively analyzed and discussed.

A1-0066

Gowth and Characteristic study of Glycine Lithium Nitrate crystal grown using Sodium Nitrate, Potassium Nitrate as an additive

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Abstract. Slow Evaporation technique is the easier way to grow crystals and work best for compounds which are not sensitive to ambient condition in laboratory. The crystals of centrosymmetric glycine in its pure form show Second Harmonic Generation (SHG) upon occlusion of guest molecule. Non-Linear Optical (NLO)materials obtained from amino acid have potential application in Second Harmonic Generation. Single crystal of glycine in the presence of small amount of Lithium Nitrate, Potassium Nitrate, Sodium Nitrate, Potassium Chloride, Potassium Bromide are good non-linear optical (NLO) materials. Crystals of glycine lithium nitrate with their non-linear optical properties have been grown in a solution by slow evaporation technique. Crystals of Glycine Lithium Nitrate are grown by slow evaporation technique and dopped with 20%, 30%, 50% and 60% of Sodium Nitrate and Potassium Nitrate. Sample surfaces and evaluation of the content ratio of doping material have been made by EDAX test, crystalinity and functional group of crystal characterized by FTIR- UV measurement studies and morphology of crystals are studied from SEM analysis.

Effect of Structural Modification on Electrical Properties Polymer Electrolytes

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Abstract. Solid polymer electrolyte (SPE) systems with poly (ethylene oxide) PEO as polymer and Rubidium Bromide (RbBr) as salt were prepared. The SPE system PEO:RbBr doped with 10 wt% of RbBr, which is stable and exhibits highest ionic conductivity of 4.02x10⁻⁶ Scm⁻¹ was structurally modified by irradiating with low energy oxygen ion beam. Ionic conductivity and dielectric properties of the SPEs are evaluated by studying complex impedance spectra. SPE irradiated with 1x10¹⁵ ions/cm² shows one order enhancement conductivity (3.61 x10⁻⁵ Scm⁻¹). The single peak in dielectric loss tangent curves indicates the fact that ion motion in the polymer network is aided by segmental motion. The decrease in the relaxation time (τ) in the irradiated SPEs shows increased segmental motion as a result of reduced crystalline phase. The decrease in the activation energy from 0.28eV (un-irradiated) to 0.12 eV (Irradiated with1x10¹⁵ ions/cm²) observed in temperature dependence studies of ionic conductivity indicates the increase in amorphous phase. X-ray diffraction graphs shows increase in peak width along with reduced peak intensity of characteristic peaks and thermal studies shows decrease in glass transition temperature (Tg) as well as melting point (T_m) in case of irradiated SPEs, both these observations support the observed enhancement of amorphous phase due to irradiation. The appearance of D-LAM band in Raman spectra further proves modification in the morphology of SPE systems.

A1-0068

Solvent phase study on conformational behavior and metal complexes of methylselenocysteine: A computational exploration

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Abstract. The conformational behavior of the zwitterionic methylselenocysteine molecule around its structurally important torsional angles was investigated in the present study. All the calculations were performed at B3LYP/6-311++G(d,p) level of theory in the solvent phase. Total electronic energies, HOMO-LUMO energy gaps, Gibbs energies, rotational constants, dipole moments, vibrational frequency and other structural parameters were systematically computed and analyzed. Further complexes of the most stable conformer with transition metals were designed in 1:2 ratio (metal: ligand). The optimized metal complexes were docked with DNA. The study reveals significant insight concerning the solvent phase conformational aspects as well as molecular properties of the conformers and the metal complexes.

Aging Effect on the Optical and Structural properties of Cr₂O₃ nanoparticles prepared by coprecipitation Method

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Abstract. The structural and optical properties and aging effect on as-grown Cr₂O₃ nanoparticles are demonstrated in this research article. Cr₂O₃ nanoparticles have been rapidly synthesizedby coprecipitation method at room temperature. The effect of aging on the growth of Cr₂O₃ nanoparticles was investigated by their crystal structure and morphological analysis were characterized by X-ray diffraction (XRD), and Scanning Electron Microscopy (SEM). Optical properties of chromium oxide were identified from the UV-visible spectroscopy. Raman is the monitoring of oxide growth which contributes to information about the chemical nature of the oxide prepared and the stress state of the material. The crystallite sizes determined by using the Scherrer's formula were found to in increase order 18.95 to 22.46 nm Cr₂O₃ powders respectively. UV-vis is spectroscopy demonstrates the energy band gap between 3.05 to 3.14 eV. This study illustrates that Chromium oxide configurations were determined from the confocal Raman scattering factor and single structure of chromium oxide nanoparticles. Hence, synthesized Cr2O3 nanoparticles are used in various biomedical fields, gas sensors, and biosensors applications.

A1-0070

Chemical Synthesis of Holmium Oxide Nanoparticles and Its Characterization

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Abstract. For the last 3 decades' researchers have showed a great interest in the study of nanosized rare earth oxide materials because of their unique structural, morphological and optical behaviour. They exhibit interesting dielectric properties, high resistivity, high dielectric constant, low dielectric loss and good chemical, thermal and mechanical stability. The literature data on the properties of Holmium oxide are rather scarce. Holmium oxide (Ho₂O₃), is an important rare earth metal oxide, and has been used as the base material in the construction of memory devices, optical materials and pH sensing films. There are many methods for the preparation of Ho₂O₃ nanoparticles such as hydrothermal method, sono chemical method, co-precipitation method, gel diffusion method, thermal decomposition etc. Because of simplicity, reduced cost, time saving and lesser number of precursors, co-precipitation method is used to synthesize nanoparticles in this work. Structural, optical, morphological, dielectric studies, ferroelectric studies are performed and presented in this work. Holmium oxide nanoparticles are calcinated at 800°C for 3 hours and various characterizations has been done. XRD analysis, SEM EDX, FTIR, UV-VIS-NIR spectroscopy analysis, Dielectric analysis, Ferro electric P-E loop analysis are performed. Structure of the Holmium oxide nanoparticle studied using X-ray diffraction analysis shows that the samples are in pure cubic phase of Ho₂O₃. The average particle size of the nano product is evaluated using the Debye- Scherrer's equation. The average particle size of raw powder is found to be 6.79nm and for calcinated powder it is 22.54 nm. In order to study the lattice strain, Williamson-Hall (W-H) plot is drawn with $4\sin\theta$ along the x-axis and $\beta\cos\theta$ along y axis and is linear fitted for the two samples. Slope and Y intercept of the fitted line represents strain and the particle size. For raw powder, the particle size is found to be 5.68 nm and for calcinated powder it is 23.4 nm. Strain of the samples is also found out. The size of nano particles obtained from the W-H plot is in close agreement with XRD analysis. Scanning electron microscopic images of the nanoparticles clearly shows polyhedron shape with few agglomerations and negligible porosity. Crystalline sizes from SEM analysis are in the range 5- 40 nm. The size of particles is in close agreement with the XRD results. EDX spectrum of the compound confirms the presence of O and Ho peaks that are related to the Ho₂O₃ nanoparticles. Only peaks corresponding to the elements of Holmium oxide is found thereby confirming the purity of the compound and the reliability of the synthesis route. The UV-VIS-NIR absorption spectrum of the sample is taken in the range 200nm to 1500nm. The optical absorption band at 300 nm in the UV region is observed which is assigned to the Ho₂O₃characteristic bond of absorption. The energy gap of the sample is found using the Tauc relation and it is found to be 3.875 eV. In order to confirm the formation of Holmium oxide from its precursors and to ascertain the various functional groups present FT-IR spectrum is recorded in the range 400–4000 cm⁻¹. A plot of the dielectric constant ε, dielectric loss tangent (tan δ) at room temperature for frequencies 100 Hz - 10 MHz is performed. The dielectric constant is large in the lower frequency region and rapidly reduces as the frequency increases, becoming almost saturated at the high frequency area. As the frequency increases, the tan δ value decreases, which appears to follow an almost straight line. Ferro electric properties of prepared Holmium oxide nanoparticles are studied at room temperature by observing polarization in the sample. The sample shows a perfect Ferro electric loop. The shape of P-E loops shows that electric dipoles are uniformly distributed inside the material. Rare earth oxides in thin film form has potential application in different microelectronic devices as thin film capacitors, thin film transistors, as insulating coatings in optical coatings, gas sensors and as protective coatings etc. Holmium oxide has excellent uses in the wavelength calibration tools as well as pyrolysis catalysts. Preparation and dielectric examination of Ho₂O₃ films fabricated in MIM or MIS structures has gained much importance. So its studies are of great importance.

A1-0071

NiCoS electrocatalysts for overall water splitting and urea oxidation for hydrogen generation Pratik M. Pataniya*, Nandini Trivedi, C.K. Sumesh

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Abstract. Designing efficient and stable bifunctional electrocatalysts via doping strategy has been extensively studied for water electrolysis. Herein, we report the one-step hydrothermal synthesis of NiCoS bifunctional electrocatalysts for alkaline water electrolysis and urea oxidation reaction. The NiCoS electrocatalyst achieves the low overpotential of 147mV@10 mA/cm2 and 244 mV@100 mA/cm2 for hydrogen evolution and 230 mV@10 mA/cm2 439 mV@100 mA/cm2 by raising the active sites and the electrical conductivity. NiCoS exhibits more accelerated HER performance with Tafel slop of 70.9 mV dec-1 owing to faster alkaline water dissociation. NiCoS bifunctional electrocatalyst needs cell voltage of 1.87 V at current density of 85 mA/cm2. Additionally, urea oxidation is regarded as substitutable process to replace the sluggish oxygen evolution reaction for green hydrogen generation owing to its much lower theoretic thermodynamic onset potential. NiCoS exhibits also exhibits efficient urea oxidation reaction on in-situ formed NiOOH active sites. Present research offers novel insights into the research for designing and preparing efficient and durable electrodes in urea oxidation applications.

Paper based flexible Photodetector functionalized by Fe-doped SnS Nanoflakes

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Abstract. Flexible photodetectors have emerged as a pivotal component in a wide array of modern technologies, ranging from wearable devices to flexible displays and advanced imaging systems. Present research demonstrates fabrication of paper-based flexible photodetector with Fe-doped SnS semiconductor channel. Pristine and Fe-doped SnS were synthesized by one-step hydrothermal technique. As-synthesized materials were characterized by Powder XRD, UV-visible spectroscopy and SEM. Paper-based flexible photodetectors were fabricated by solvent-free hand print method. These flexible photodetectors show excellent response over broad spectral range from visible to NIR, with maximum responsivity value 10.8 mA/W, and specific detectivity 1.13 x 10¹⁰ Jones. The current study supports a substantial advancement in the design of reliable, flexible, and large-area optoelectronic devices.

A1-0073

Green Synthesis and Characterization of Silver (Ag) and Zinc Oxide (ZnO) Nanoparticles Using Rubia Cardifolia - A Comparative Review

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Abstract. Metal and metal oxide Nanoparticles has gathered tremendous scientific interest owing to their diverse applications in the field of medicine, bio-sensing, catalysis, agriculture and the environment. Nanoparticles synthesis using various physicochemical methods generates toxic, hazardous by-products, which pose health and environmental risks. To lessen these risks, green synthesis approach using plant extracts has been most preferred to synthesize nanoparticles. Green synthesized nanoparticles have particles with unique characteristics of high bio-availability, nontoxicity, large surface area and high dispersion. During last decades, green synthesized Silver (Ag) and Zinc Oxide (ZnO) nanoparticles have attracted enormous interest in various fields of science and technology. This review focuses on the mechanism of green synthesis of Silver (Ag) and Zinc Oxide (ZnO) nanoparticles using Rubia Cardifolia plant extract such as leaf, stem, root etc. The results of characterization techniques such as Powder X-ray Diffraction (PXRD), Scanning Electron Microscopy (SEM), Fourier Transform Infrared (FTIR) spectroscopy, Energy Dispersive X-ray (EDX) analysis and UV-Visible spectroscopy for green synthesized Silver (Ag) and Zinc Oxide (ZnO) nanoparticles using Rubia Cardifolia have been compared. Overall, it was found that green synthesized Silver (Ag) and Zinc Oxide (ZnO) nanoparticles using Rubia Cardifolia have Face Centered Cubic structure and Hexagonal Wurtzite structure respectively with semiconducting property.

Utilization of Biogenic Green Tea Extract for the Eco-Friendly Synthesis of Bismuth Vanadate: Elucidation of Photocatalytic Efficacy in Environmental Remediation

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Abstract. The contemporary scientific picture focuses on resolving the challenge associated with the fundamental energy dilemma. At the moment, photocatalytic water splitting, solar energy, and organic dye degradation under visible light are potential ways to deal with these problems. Nanocrystalline bismuth vanadate has gained popularity in recent years due to its potential for energy conversion and eco-friendliness. Herein, we report the phytoextract routed synthesis of bismuth vanadate nanoparticles (BVNPs) using green tea extract as a fuel and its characterization using various analytical and/or spectroscopic techniques for the assessment of physicochemical and structural properties. Further, bismuth vanadate nanoparticles were characterized by powder XRD, SEM, HRTEM, FTIR, EDX, Raman spectroscopy, and photoluminescence spectroscopy (PL). The XRD results confirmed the formation of monoclinic bismuth vanadate. The formations of BiO & VO₄³⁻ vibrations were ascertained from FT-IR data. The morphology of hallow internal structural micro entities was confirmed by SEM. The key to our investigation is a determination of the BVNPs' inherent photocatalytic efficacy, which results from their successful separation of photogenerated charge carriers. The experimental results show that the BVNPs have a remarkable ability to degrade organic molecules when exposed to visible light, with an amazing degradation yield of 98.3% over a period of 120 minutes. To expound on the mechanistic underpinnings, a cogent elucidation is offered, encompassing the photodegradation of model organic pollutants, namely methylene blue dye and rhodamine B. The profound efficacy demonstrated by the photocatalytic activity of the synthesized BVNPs serves as a foundational element affirming their viability to yield significant advancements pertinent to the domain of sustainable energy harnessing and the rectification of environmental perturbations.

A1-0075

Sustainable Phytofabrication of anatase TiO₂-decorated g-C₃N₄ Nanocomposites via *Hibiscus rosa-sinensis* for Enhanced Photocatalytic Degradation of Rhodamine B & Bisphenol A

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Abstract. Contemporary environmental concerns center around dye pollution, stemming from industries like textiles, which discharge hazardous dyes into waterways. Nanotechnology offers a promising solution by enabling the development of advanced nanomaterials for efficient dye degradation, addressing this pressing ecological challenge. In the current study, anatase TiO₂ nanoparticles were synthesized using a hibiscus leaf extract, and the synthesis of TiO₂-doped g-C₃N₄ nanocomposites (changing 0.5 mM, 1.0 mM, 1.5 mM, and 2.0 mM) by thermal polymerization. Here, the proposed study used a variety of analytical methods to characterize the as-prepared TiO₂ nanoparticles and TiCN nanocomposites, including UV-Vis spectroscopy, a diffraction pattern (XRD), SEM coupled with EDX analysis, higher temperature stability (TGA), and paramagnetic resonance character (EPR). When compared to g-C₃N₄, the TiCN (1.5 mM) nanocomposites had improved shape, surface area, and the ability to absorb visible light. In comparison to g-C₃N₄, the TiCN (1.5 mM) nanocomposite had improved shape, surface area, a stronger ability to absorb visible light, and a smaller band gap. Utilizing rhodamine B and bisphenol A, the sample designated as TiCN (1.5 mM) revealed improved performance in terms of adsorption and photocatalytic activity. Additionally,

compared to g-C₃N₄, the TiCN (1.5 mM) composite had good stability throughout four cyclic runs, suggesting its potential use in reducing the impact of organic wastewater pollutants.

A1-0076

Green Synthesis of Silver Nano Particles from The Extract of Psidium Guajava, Musaceae, Azadirachta Indica and Mangifera Indica

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Abstract. The physicochemical and optoelectronic properties of metallic nanoparticles are strongly dependent on the size and size-distribution, but also nanoparticles shape contributes significantly to the control of their properties. A rapid, cost-effective and eco-friendly approach to obtaining stable silver nanoparticles in aqueous media, and at room conditions, has been established, employing fruit extract as the reducing agent. UV–visible spectroscopy is the technique to check formation and stability nanoparticles which produced by psidium guajava, musaceae, azadirachta indica and mangifera indica. From the evidence of Ultraviolet-Visible spectroscopy different sizes of Silver nanoparticles were formed when the juice volume, reaction temperature, and reaction time were altered with respect to 0.001 M silver nitrate solution.

A1-0078

A mini review on the anode buffer layers used in organic light emitting diodes

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Abstract. Research on organic light emitting diodes (OLEDs) are recently increasing due their unique advantages over inorganic devices. To explore upto the technology, there is a need to understand the basic device physics of OLED. The basic device physics of the device consists of basically three steps i.e. device structure, device mechanism and device characteristics & their parameters. Device structure of OLED typically consist of three basic layers but there are several intermediate layers are used to enhance device efficiency. Anode buffer layers are used to are used to reduce the interface barriers present at anode/HTL interface. Here, in in this paper different used anode buffer layers are reviewed.

Investigation of structural and magnetic properties of Cobalt doped Nickel Ferrite sintered at different temperatures

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Abstract. Currently, magnetostrictive materials are receiving a lot of attention due to their widespread use in technical applications of Magnetoelectric energy harvesting. In modern magneto mechanical stress sensors, actuators, and torque sensors, the magnetostrictive ferrites are commonly used. In this investigation, we studied the properties of $Ni_{0.5}Co_{0.5}$ $Fe_2O_4(NCFO)$ nanoparticles prepared using a solgel synthesis process and sintered at different temperatures 1100 °C, 1200 °C and 1300 °C. The XRD patterns of NCFO samples confirm the crystalline nature of the material. The lattice parameters are found to decrease with increase in sintering temperature. As the crystallite size increases with increasing temperature the lattice parameter decreases. The microstructure of the different samples was analyzed using a field emission scanning electron microscope. Bond angles and bond lengths between the atoms were estimated using the Rietveld refinement technique. A clear effect of sintering temperature has been observed in the bond angles between the atoms. Unit cell of the compounds are generated with VISTA software and the results are discussed in the paper.

A1-0080

Thermal Management of Pouch-Type Li-Ion Batteries: A Computational Analysis

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Abstract. The transition toward electric vehicles (EVs) powered by lithium-ion batteries (LIBs) has gained momentum due to their potential to reduce fossil fuel dependence and mitigate environmental impacts. However, the thermal management of LIBs remains a critical challenge affecting their efficiency, longevity, and safety. In this study, we employ ANSYS numerical simulation software to investigate the thermal behavior of pouch-type LIBs used in commercial applications under various discharge rates. To analyze thermal behavior, we utilize the empirical model proposed by the Multi-Scale Multi-Dimensional (MSMD) group's researchers Newman, Tiedemann, Gu, and Kim. The simulations are carried out at different C-rates (1C, 2C, 3C, 4C, 5C, 10C, and 15C), and detailed contour plots of phase potential for both negative and positive tabs are presented. Our results indicate that the battery's maximum surface temperature is directly related to the discharge rate, with higher C-rates leading to elevated temperatures. To address this thermal issue and enhance discharge capacity, we introduce a water-based liquid cooling system and evaluate its effectiveness in reducing the maximum cell surface temperature. This study plays a pivotal role in advancing the development of innovative cooling systems for LIBs, with the aim of optimizing battery performance and ensuring safe operation. As the electric vehicle industry continues to grow, addressing thermal management challenges will be paramount in achieving sustainable and efficient EV technologies.

Exploration of optical properties of novel and flexible CS-GO composites

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Abstract. Extraordinary features of bio-degradable Chitosan (CS) and 2-D nano-filler (Graphene Oxide: GO) has motivated us to study the optical properties of newly developed polymer composites: CS-GO. For the synthesized CS-GO composites via usual solution mixing technique, we have explored optical properties in terms of absorption spectra, optical band gaps (direct and indirect both), refractive index and Urbach energies. According to the outcomes, it has been noted that the amount of 2-D nano-filler has capability to reduce the band gap; while the refractive index and Urbach energy is increased significantly on increasing amount of GO.

A1-0082

Effect of Solvent on the Performance of Dye Sensitized Solar Cells Using Natural Dye as Sensitizer

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Abstract. The study explores the role of different solvents in the efficiency of solar cells manufactured from natural dyes and evaluates their optical and electrical performance. The UV–Visible absorption spectroscopy were used to analyze the optical properties. The photovoltaic perfomance of DSSCs were evaluated at light intensity of 100 mAcm^{-2} . Short-circuit current (i_{SC}) ranged from 1.209 to 1.792 mA, open-circuit voltage (V_{OC}) ranged from 1.608 to 1.941 V, and fill factor ranged from 0.45 to 0.64. The power conversion efficiency varies from 1.297 and 1.52 %. This paper briefly describes the extraction techniques of these natural dyes and their performance in various solvents.

Doping Effect CuO Nanoparticles On Structural, Optical and Morphological Properties of Polypyrrole

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Abstract. Herein, we presented the effects of CuO nanoparticles on the structural, optical and morphological properties of polypyrrole (PPY). Pure PPY and PPY-CuO nanocomposites were prepared via chemical oxidative polymerization technique in sulphuric acid aqueous solution. Structural, optical and morphological properties of the synthesized materials were characterized using the X-ray diffraction analysis (XRD), ultraviolet-visible (UV-vis.) spectroscopic and field emission scanning microscopy (FESEM) techniques respectively. The amorphous nature of the pure PPY was confirmed by the structural study and PPY-CuO also shows the same nature without any considerable change. Optical study shows the two absorption peaks at 256 and 450 nm in pure PPY and PPY-CuO shows the slight shifting in the absorption peaks due to the doping. Morphological study agreed with the XRD study and shows the amorphous nature.

A1-0084

Computational Study of Electrochemical CO2 Reduction on Two-dimensional TiB2 Monolayer Durvesh Patil ¹ and Aarti Shukla ²*

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Abstract. The production of organic molecules from CO₂ is extremely desirable from both an energy and environmental standpoint. High-performance catalysts are necessary to accomplish such a desirable outcome. In this paper, TiB₂, a two-dimensional (2D) transition metal diboride, has been used to examine the CO₂ reduction pathways such as formic acid, methanol, and CH₄ using density functional theory. TiB₂ monolayers with inherent transition metal terminated surfaces have strong catalytic activity for converting CO₂ selectively to HCOOH with a 0.56 eV overpotential. Further, the electronic properties and charge differences are also investigated to gain knowledge regarding thnature of adsorption at catalytic surface. These new 2D materials are especially appealing due to their excellent catalytic performance.

Electrochemically deposited metal oxide thin film for competitive enzymeless detection of neurotransmitters

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*Corresponding author: fahmed.phys@aliah.ac.in (Sk. F. Ahmed), nilsci@yahoo.co.uk (NM) Abstract. Dopamine and serotonin are the two well-known electroactive neurotransmitters that belong to the family of catecholamines. Dopaminergic and serotonergic systems play vital roles in neuromodulation in human physiology and in the central nervous system also. So, their deficiencies can cause some serious neurological disorders and also affect emotional behaviour like regulation of mood, stress, and depression etc. An electrochemical technique was adopted to deposit CuO/Cu2O bulk heterostructure thin film on indium doped tin oxide (ITO) coated glass substrates aiming to discover its non-enzymatic electrochemical sensing performance of the two neurotransmitters, viz. dopamine (DA) and serotonin (ST). All structural and morphological characterization including XRD, FT-IR, FESEM, AFM were carried out for the deposited material, followed by detailed electrochemical analysis toward the sensing of dopamine and serotonin in phosphate buffer solution. XRD pattern revealed the presence of both CuO (monoclinic) and Cu2O (cubic) phases in the deposited thin film. Structural investigation was further supported by FT-IR and it also confirms to the existence of both CuO and Cu2O phases. The morphological analysis was carried out using FESEM and AFM. High magnification FESEM micrograph revealed the compactness in surface that made up of closely packed agglomerate particles whereas, the good value of surface roughness (28.42 nm) getting from the AFM analysis exposing more active sites for better electrode – electrolyte interaction. The sensitivity of the electrode was found to be 9.22 µA µM⁻¹ cm⁻² with a limit of detection (LoD) of 0.388 µM for dopamine in the electrochemical analysis. Whereas, for serotonin, the sensitivity and LoD values were 1.18 μAμM⁻¹cm⁻² and 8.11 μM, respectively. Further in the mixture of dopamine and serotonin the modified electrode showed sensitivity (5.39 µA µM⁻¹ cm⁻²) and LoD (0.50 µM) more likely as pure dopamine. These results clearly indicated that the CuO/Cu2O bulk heterostructure electrode is a better candidate for the electrochemical detection of dopamine, whereas its serotonin sensitivity was average. This makes the electrode more selective to dopamine.

A1-0086

Computational Study of Ga Doping on the Structural and Electronic Properties of Stanene Anver Aziz^{1,a)} and Indu Barak^{2,b)}

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Abstract. Stanene, a two-dimensional honeycomb-like structure composed of tin atoms, has gained significant attention in the field of materials science due to its intriguing properties, particularly its topological nature as a quantum spin Hall insulator. Its potential applications in spintronic devices have been a subject of interest, but its inherent gapless nature poses limitations for practical use in certain electronic applications. To overcome this limitation and enhance its usefulness in spintronics, density functional theory calculations were conducted to investigate the effects of Ga (gallium) doping on the structural and electronic properties of stanene. Density functional theory calculations were performed to investigate the effect of Ga doping on the structural and electronic properties of stanene. Stanene, a two-dimensional honeycomb-like structure composed of tin atoms, exhibits gapless characteristics. However, its potential for applications in spintronic devices is limited due to its gapless nature. In this study, Ga atoms were substituted into the tin vacancies of stanene to explore the band gap tuning in this material. The results show that 3% Ga-doped stanene exhibits a sizable band gap, whereas pristine stanene remains gapless. Further analysis of the band structure reveals a shift in the Fermi level in Ga-doped stanene, indicating changes in its electronic properties. These findings provide a theoretical basis for utilizing Ga-doped stanene in next-generation spintronic devices.

Structural, morphological, and photocatalytic properties of Mn-doped V₂O₅ Prashant Choudhary^{1,b)}, Vikas Dhiman^{1,2,c)}, Abhishek Kumar^{1,d)}, Neha Kondal^{1,a)}
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Abstract. The primary global problem of the twenty-first century is the lack of freshwater and the proliferation of various pollutants, such as microorganisms, heavy metals, and dyes. As a result of the world's industrialization, which is accelerating at an alarming rate, dyes and pigments have increasingly become a common component of wastewaters due to their extensive usage across numerous sectors, including paper production, textile dyeing, cosmetics, paints, and food processing. Over 700,000 tones of synthetic dyes are produced annually, and more than 15% of these dyes are released into the water. Furthermore, it is claimed that just 47% of synthetic colors are biodegradable. Therefore, the removal of dyes from industrial effluents is an important environmental concern as most of them are nonbiodegradable, toxic, and can even cause cancer. One of the most prevalent environmental remediation technologies that provide a safe and efficient way to deal with organic dyes from wastewater is semiconductor photocatalysis. In this technique, hazardous dyes are converted into nonharmful by-products without creating any waste. Advanced oxidation processes like photocatalysis involve complete photo-mineralization or oxidation of harmful textile dyes by the generation of hydroxyl and superoxide radicals that react with most organic substances and mineralize them into CO₂, H₂O, and smaller hydrocarbons without intermediate byproducts. The present investigation describes the synthesis of manganese-doped V_2O_5 (Mn_x $V_{2-x}O_5$ with x = 0.00, 0.01, 0.02, 0.03, and 0.04) and its application in photocatalytic degradation of methylene blue (MeB) dye. Mn_xV_{2-x}O₅ samples were synthesized using a solid-state reaction followed by calcination in a muffle furnace at 450 °C for 6 h. The prepared samples were Mn_xV_{2-x}O₅ samples were characterized for their structural and morphological characteristics using powder X-ray diffraction (XRD) and scanning electron microscopy (SEM), respectively. The X-ray diffraction shows that Mn doping results in the variation of crystallite size due to strain induced in the prepared samples which is calculated by the Stoke-Wilson relation. The SEM images illustrate the surface structure of both the pristine and Mn-doped V₂O₅, revealing the polycrystalline characteristics of the prepared nanoparticles. The photocatalytic performance of Mndoped V₂O₅ samples was investigated by decomposing methylene blue dye to explore the potential of $Mn_xV_{2-x}O_5$ for environmental remediation. The results show that Mn-doped V_2O_5 has a good ability for photocatalytic dye degradation with a high reaction rate constant.

A1-0088

Tunnel FET and Bilayer Van der waal (vdW) Source Tunnel FET, A Comparative Study

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Abstract. Tunnel Field Effect Transistor (TFET) has proved to be a promising device in case of VLSI and ULSI circuit design. It is a good low power device in terms of minimum short channel effects and random dopant fluctuation in comparison to MOSFET. Semiconductor device production is devoted to support technology platform in two device types namely 1) high performance logic and 2) low power logic and More Moore Roadmap provides a view of enablement of continued scalling to make trends of improvement of device in low power possible. In spite of low Subthreshold Swing (SS) low ON current of conventional TFET exhibits a real challenge. Following the trend here in this paper we introduce an approach of increasing I_{ON} of TFET composed of Black Phosphorene(BP) homojunction by Van der waal (vdW) stacking in source region and is compared with its monolayer counterpart. Switching behavior is also studied and compared.

Smart Materials: Properties and Applications

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Abstract. Due to their receptiveness to environmental stimuli like stress, light, temperature, moisture, and electric or magnetic fields, smart materials play a significant role in our lives, covering a variety of sensing and actuation applications in healthcare. Shape memory alloys, magneto-rheostatic materials, piezoelectric materials, and electro-rheostatic materials are a few examples of these materials. Shape memory properties provide an especially tempting glimpse into the field of material science and allow for the possibility of novel functions in all kinds of materials. Smart materials mainly concentrate on the shape effects of memory and pseudo-elasticity. Due to their mechanical properties, smart materials are highly sought-after for numerous applications in biology. Smart materials are used in a variety of fields, such as robotics, aircraft, keyboards, biomedicine, etc. Smart materials are used in a variety of fields, such as robotics, aircraft, keyboards, biomedicine, etc. Additionally, these materials can be used to create biofuel-using devices that collect biomechanical energy from human motions, environmental factors, or body heat. According to studies, smart materials are always more biocompatible than traditional stainless steel and other implant materials alloy. Smart-materials are widely thought to be a potential aid for tumor detection, diagnosis, and treatment. Cancer is still the leading cause of death and a significant barrier to extending life. The nano-drug delivery approach is crucial to the use of smart materials in the treatment of cancer.

A1-0090

Synthesis and Electrochemical study of Ti₂GaN electrode material.

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Abstract. This article presents the synthesis of Ti_2GaN nanoparticles using Electrochemical method. Performance of the synthesized nanomaterial was further characterized by using the X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), UV-Visible Spectroscopy(UV-VIS) and Cyclic voltammetry (CV) studies. It has been observed from XRD that the sample show a simple cubic structure. The crystallite size of sample was in the range of 6.76 nm-30.71 nm. The FT-IR bands of TiO_2 and GaN show a strong interaction between TiO_2 and GaN. From UV-VIS studies, the absorption band for Ti_2GaN are around ~ 208 nm, ~ 233 nm, ~ 258 nm, ~ 321 nm. The Electrochemical performance of active material using Potassium hydroxide as an electrolyte is analysed. The Specific capacitance for synthesized nanomaterial at 1 A/g was found to be 16 F/g.

Analysis of Novel Transistors on Energy Saving Approaches

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Abstract. The entire planet is facing the challenges regarding energy shortage. Due to massive population, pollution and excessive growth of industrialization, scarcity of natural resources has been occurred. As the result, the whole world is searching the new technology for energy sufficient products. In this work, novel Junctionless Field Effect Transistor (JLFET) with gate engineering applications has been discussed for low power and energy saving issues. Due to device miniaturization, implantation of junctions with doping concentration ranges up to 10^{19} to 10^{20} cm⁻³ within the nanoscale gate length is a challenging task. Researchers have provided the innovative idea of JLFET for replacement of conventional transistor (CT). The results show that JLFET are highly immune to short channel Effects (SCEs) than CT. The analysis of JLFET has been provided to support the researchers for product development in ULSI design.

A1-0092

Electrical Resistivity and Structure of Some Cu-Zr Metallic Glasses

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Abstract. The electrical properties of metallic glass are closely related to their unique amorphous structure. Fully understanding of electrical properties of metallic glass and their composites requires investigation of resistivity, thermo power and their structure. In this paper we have obtained partial structure factors of four glasses of Cu-Zr system. We have also computed electrical resistivity at 300K for each glass using Faber-Ziman formalism. The variation of resistivity due to change in concentration in series of Cu-Zr system have also been studied. Theoretical studies were performed using pseudopotential method which has been capable of explaining in past various properties like electrical, superconductivity, transport etc. for metallic glass. Four metallic glasses, Cu₂₅Zr₇₅, Cu₃₀Zr₇₀, Cu₄₀Zr₆₀, Cu₅₀Zr₅₀, were chosen for study. Calculated Resistivity has been found to be in good agreement with the experimental values provided in the literature. The graphs of partial structure factors of all the glasses have been obtained and discussed. Partial structure factors are able to produce correct resistivity value of corresponding glass so we consider these partial structure factors may form basis of calculation of other properties of these glasses. The composition dependent linear equation for low concentration of Cu has also been provided.

Unlocking Enhanced Quantum Capacitance in Functionalized WS2 and WSe2 Supercapacitor Electrodes

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Abstract. In this work, we investigated the electronic structure and the quantum capacitance of a set of functionalized WS2 and WSe2 monolayers. The functionalizations have been done by using different ad-atom adsorption on these monolayer. Density functional theory calculations are performed to obtain an accurate electronic structure of ad-atom doped WS2 and WSe2 monolayer with a varying degree of doping concentration. Subsequently, the quantum capacitance in each functionalized system was estimated. A marked quantum capacitance above $100\mu F/cm^2$ has been observed. Our calculations show that the quantum capacitance of these monolayer is significantly enhanced with substitutional doping with transition metal ad-atoms. The microscopic origin of such enhancement in quantum capacitance in this system has been analyzed. Our DFT-based calculation reveals that the generation of new electronic states at the proximity of the band-edge and the shift of Fermi level caused by the adatom adsorption results in a very high quantum capacitance in the system.

A1-0094

Anticancer, Antioxidant and Antimicrobial Activity of Silver Nanoparticles Synthesized Using Fruit Extract of *Artemisia Maritima*

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Abstract. In this paper, we wish to report a simple, convenient and green synthesis of silver nanoparticles employing aqueous extract from fruits of Artemisia maritima. The aqueous solution of metal ion was treated with aqueous fruit extract from medicinal plant Artemisia maritima, stirred for few minutes and left overnight at room temperature. The nanoparticles thus formed were filtered and dried in an oven. Biosynthesized silver nanoparticles were characterized by UV-Visible, IR, XRD and Scanning Electron Microscopic techniques. The XRD, SEM, UV and FTIR results were found to be promising. This green method can be used for the synthesis of metal nanoparticles by retaining their biomedical utility. Biosynthesized silver nanoparticles further evaluated for their anticancer, antibacterial and antioxidant activity. This green method is very handy for the synthesis of metal nanoparticles and devoid of toxic chemicals and by-products, offering numerous benefits of compatibility for pharmaceutical and biomedical applications.

Electron Beam Deposited Thin Titanium Films and Its Thermal Oxidation to Form Rutile TiO₂ Thin Films

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Abstract. Titanium is a very useful biocompatible metal which is widely used in the biomedical fields for manufacturing boneanchoring devices as well as cardiac valves and accessories. Compared to other implanting metals, Ti is found advantages for its higher strength and fatigue-resistanceas well as its excellent resistance against corrosions. The absorption mechanism of proteins and interaction pathway of host tissue with the Ti surface is very crucial for any clinical applications. However, to examine the protein interactionsuccessfully, a smooth surface morphology of Ti is required to biomimicry the model system. In addition, Ti film surface morphology can significantly influence its surface oxidation process. Apart from Ti films, titanium dioxide (TiO₂), based nanostructures are extensively used in sensors, solar cell, and energy storage devices. Hence a detailed understanding of the Ti film formation and its controlled oxidation process are of high scientific as well as technological interest.

Within this work, we will studyabout the formation of thin Ti film and its thermal oxidation process. High purity Ti was deposited on the quartz substrates using an electron beam evaporation technique, conducted under a high vacuum condition keeping the base pressure below ~10⁻⁵ mbar (HindHighVac). In order to form oxide layers, controlled thermal oxidation of the as-deposited Ti films has been performed in air ambient condition, using a muffle furnace (TEMPCON). Thermal oxidation was conducted at various temperatures for different duration. Structural, morphological, chemical, optical and electrical properties of these oxide layers have been investigated using various surface characterization techniques such as x-ray diffraction (XRD), scanning electron microscopy (SEM), Raman spectroscopy, and x-ray photoemission spectroscopy (XPS). Formation of rutile TiO₂ phase is confirmed from XRD and Raman spectroscopy whereas SEM imaging suggests a smooth and homogeneous growth of Ti and oxide layers, appear with a nanometer scale granular surface morphology. All finding are explain in terms of surface thermodynamics and chemical reactivity.

A1-0096

Fabrication of CrSi₂ Thin Films in Magnetron Sputtering and their Thermoelectric Properties

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Abstract. Using modern spectroscopic methods, $CrSi_2$ thin films of different thicknesses obtained by the solid-phase ion-plasma method on the Si surface were investigated. The composition, surface morphology, cross section, temperature dependence of resistance, Seebeck coefficient and power factor of the thin films were studied. It was found that the Si surface is completely covered with an amorphous $CrSi_2$ film from a thickness of ~ 42 nm. After heating the $CrSi_2/Si$ system at $t \approx 480^{\circ}C$, a homogeneous polycrystalline $CrSi_2$ film is formed. Their values are slightly different for $CrSi_2$ films of different thicknesses. In particular, with the increase of T, it was found that the resistance r of the polycrystalline film decreases and the Seebeck coefficient S increases. The non-linear variation of resistance r, Seebeck coefficient S and power coefficient P of $CrSi_2$ film of different thicknesses with increasing temperature is shown.

Facile preparation of ZnO nanoflakes (2D) ink for printed electronic devices and their morphological characterization

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Abstract. Two- dimensional (2D) Zinc oxide (ZnO) nanoflakes (NFs) is the most studied ultimate structure because of its ease of preparation, high sensitivity, improved selectivity, fast response and low cost. ZnO NFs have been successfully synthesized by zinc acetate and sodium hydroxide via simple, single step Sol-gel technique. After dispersing it into ethanol 2D ZnO NFs ink was prepared which is highly favorable for developing high performance, large area printed electronic devices, photodetectors, solar cells and sensor applications. In order to have a reliable characterization, systematic studies including Scanning electron microscopy, EDAX analysis have been carried out for as prepared ZnO NFs. The XRD spectra confirms the wurtzite crystal structure and SEM images confirms the sheet morphology of as prepared ZnO NFs.

A1-0098

High performance ZnO Quantum Dot/Graphene/Hexagonal Boron Nitride/GaN Heterostructure Based UV Detector

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Abstract. High performance ultraviolet (UV) photodetectors are in great demand for strategic applications such as military, flameout protection, missile flame detection and many other applications based on different sub bands of UV detection. Conventional UV detectors are constrained by size, high dark current noise and cost. There is a need for high performance, compact size and less expensive UV detectors. In this paper, a ZnO quantum dot photo-doped graphene/hexagonal Boron Nitride (hBN)/ GaN substrate heterostructure based UV detector is designed, simulated and analyzed for its performance prediction. Electrical and optical characteristics of the device are obtained using a device simulator. The hBN layer at the graphene/GaN interface is used to decrease the dark current. ZnO quantum dot layer deposited on the graphene/hBN/GaN heterojunction help in increasing the responsivity of the device due to its long trapped-charge life time. This detector provides high responsivity in the deep UV to UVA region (100 nm-350 nm) compared to the devices without hBN and ZnO quantum dots layers.

Vibration behavior analysis of functionally graded annular piezoelectric plate for free-free boundary conditions

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Abstract. Functionally graded piezoelectric material has very enormous application in the field of engineering and science. It is very useful for smart device like micro electric mechanical system, nano electro mechanical system. In the present work the effect of diametric ratio has been observed for functionally graded piezoelectric circular plate for free-free boundary conditions. d₁₅ effect has been utilized for exited shear induced flexural vibration. Due to complex nature of shear vibration these effect is less utilized. Plate has been readily polarized and electric effect is applied along the thickness direction.

A-0100

Absorbance and Fluorescence Studies to Investigate Nickel Oxide Nanoparticles-Glucose Interaction

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Abstract. In the present study, hydrothermal technique is utilized to prepare nickel oxide nanoparticles. Synthesized nickel oxide nanoparticles having cubic structure with average crystallite size about 17 nm is observed by X-ray diffraction analysis. Intense absorption peak at around 324 nm was noticed by UV-VIS spectroscopy corresponding to band gap of ~ 3.91eV. Interaction of prepared nickel oxide nanoparticles with glucose at different concentrations is monitored to study the effect on the absorption and fluorescence spectra. Substantial changes in the fluorescence/ absorption intensity are seen, demonstrating the strong interaction between glucose and nickel oxide nanoparticles. Linear behavior is observed between the change in absorption intensity as a function of concentration in double reciprocal plot. However, exponential dependence between the change in fluorescence intensity and concentration of NiO nanoparticles in glucose solution is seen.

Existence and Stability of Discrete Intersite Bright Solitons in Bose Einstein Condensates in Parabolic Trapped Optical Lattices

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Abstract. We consider intersite discrete bright solitons in one-dimensional Bose-Einstein condensate in parabolic trapped optical lattice. Analytical and numerical calculations are performed to determine the existence and stability of bright solitons. Analysis is based on continuous Gross-Pitaevskii equation and discrete nonlinear Schrodinger equation. It is observed that the strength of external magnetic trap can change the stability of bright solitons. Stability windows of bright solitons are presented and stability approximations are derived using perturbation theory, with their numerical results.

A1-103

Computational Investigation on Electronic Properties of Ag Doping in Cu₂ZnSnSe₄ Solar Absorber Material

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Abstract. Kesterite Cu₂ZnSnS₄(CZTS) and Cu₂ZnSnSe₄ (CZTSe) chalcogenide compounds are highly promising for the low-cost and high-efficient thin film solar cell technology. Herein, we have introduced Ag as a cation site substitution to passivate and explore the optoelectronic properties of CZTSe absorber material. The electronic properties of Ag doped (0, 10, 20 %) CZTSe compounds were investigated using the highly accurate Tran–Blaha-modified Beck and Johnson (TB-mBJ) potential by the full potential linear augmented plane wave method (FP-LAPW) via Wien2K code. Electronic structure calculation predicts that these chalcogenide compounds are direct band gap semiconductors. The total and partial density of states (DOS) of all the compounds analyzed and reported. It is further confirmed from present calculation that Ag incorporation (10%) in CZTSe provides the higher total DOS as compared with pristine and 20% Ag doped CZTSe system.

Structural and Optical Analysis of NaSrPO4 Nanostructure as Synthesized by Sol-Gel Technique

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Abstract. An orthophosphate material, NaSrPO4, was successfully synthesized by using sol-gel technique. X-ray diffraction analysis by using Rietveld refinement used to verify the single phase purity of NaSrPO4. The refinement was carried out in orthorhombic cubic crystal structure with space group *Pnma*. The obtained lattice parameters were a = 20.41 Å, b = 5.43 Å, c = 17.25 Å. The luminescence results show that NaSrPO4 excited at the wavelength at 285 nm exhibits an intense broad emission spectrum range from 380-500 nm. All these characteristics suggest that the NaSrPO4 is applicable for optoelectronic devices.

A1-0105

Nanotechnology: A holistic approach to decontaminate polluted groundwater

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Abstract. It is a much known fact that water is an essential commodity for human health, agriculture industry and sustainability of the earth's Ecosystem. Rapid economic and industrial growth has caused more water consumption. Faster industrialization not only created pressure on water resources but also on its quality. The activities of industries cause many rivers, lakes and groundwater to be polluted by heavy metals like manganese, arsenic and iron. Among all groundwater pollutants, metal ions such as Zinc, Mercury, Lead, Nickel, Arsenic, Chromium and Cadmium have high lethal and nonbiodegradable properties and can cause several health problems in animals and human beings. Thus removal of such toxic metal from groundwater is becoming a decisive issue. In order to remove heavy metals from polluted water, several methods have been established. Although traditional sorbents could remove heavy metal ions from groundwater, the low adsorption capacities and efficiencies limit their application deeply. To solve these defects of traditional sorbents, Nano-materials are used as novel ones to remove heavy metal ions in groundwater. With the rapid development of nanotechnology, there has been a great deal of interest in environmental applications of nanomaterial that are excellent adsorbents and catalysts. Nano materials offer significant improvement with extremely high specific surface area, numerous associated sorption, low temperature modification and short intra-particle diffusion distance. Extensive research has been carried out to remove heavy metals from groundwater by developing and using various Nano materials. In addition to synthesized nanoparticles, modified nanoparticles were also synthesized to improve the adsorption capacity of nanoparticles.

A Review on luminescence spectroscopy of oxide nanopowders trivalent lanthanide ions doped garnet

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Abstract. In this review, we deal with the structural investigation of the garnet family of oxide materials activated with trivalent lanthanide ions, in the nanocrystalline form. In particular, attention is devoted here to the important garnet hosts; structure and luminescence spectroscopy are presented and discussed, with particular emphasis given to the possibility of obtaining efficient luminescence from trivalent lanthanide ions at the nanoscale, and to the potential and envisaged technological applications of this class of materials.

A1-0107

On the effective permittivity of the multicomponent dielectric-dielectric nanocomposite structures

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Abstract. In modern photonics, the calculation of effective optical properties of composite materials is of significant interest because it allows to predict the characteristics of the resulting material and provides a deeper understanding of the basic physical processes. There is no doubt that any research performed in this field is greatly Interesting as numerous aspects still remain enigmatic. The present article considers a multicomponent nanodispersed structure consisting of randomly oriented ellipsoidal nanoparticles in a matrix with a permittivity ε_m . Using the Maxwell-Garnett and Bruggeman models, the dependence of the effective dielectric permittivity of such a structure on the orientation of particles in an external field and the coefficient of volume filling of the medium with particles was studied.

B1-0003

Gamma Irradiation Effects on Structural, Thermal and Optical Properties of *CSR2* Silk Fibroin Films

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Abstract. In this work *Bombyx mori* silk fibroin (SF) films were prepared by solution casting method. Gamma irradiation of protein biopolymer films were carried out in dry air at room temperature using Co – 60 source, and radiation doses are in the range of 0-300 kGy. The unirradiated and irradiated films were characterized by X-ray diffractogram (XRD), thermogravimetric analysis (TGA) and ultra violet visible spectroscopy (UV-Vis). The observed interesting results have been tried to be correlated with structural, thermal and optical properties.

B1-0004

Review On A Novel MXene Based Transition Metal Oxide (TMO) Nanocomposite Electrode Materials For High Performance Supercapacitors

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Abstract. MXene, a unique 2D layer material that has great potential in energy storage fields, have attracted significant attention due to excellent metal conductivity, redox reaction active surface and hydrophilic nature. So it has been considered as promising materials for the development of supercapacitor electrode material as it exhibits high power density and low energy density it is presently inferior to the limited electrochemical performance exhibited by the conventional electrode materials. To further improve the electrochemical performance of MXene materials the variety of transition metal oxides (TMO) nanocomposites are being prepared by using hydrothermal synthesis method by the self-assembly process. This review emphasizes a simple and efficient hydrothermal synthesis method for developing high- performance MXene-based TMO nanocomposites electrodes materials for supercapacitors. Furthermore, electrochemical performance, electrical conductivity, specific capacitance, cycling stability and structural stability of different materials is discussed. Finally, we discuss the recent trends in development of MXene based electrode materials and future prospects of improvement in the performance of the supercapacitors.

Thermo-physical Properties Of Ag-Al-Au-Cu Quaternary Liquid Alloy

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Abstract. Thermodynamic and surface properties of Ag-Al-Au-Cu quaternary liquid alloy were estimated at 1573 K, 1673 K, 1773 K and 1873 K using General Solution Model (GSM), Toop model and Kohler model. The energy interaction parameters of liquid binary subsystems of Ag-Al-Au-Cu for Excess Gibbs free energy of mixing were optimized in the framework of Redlich-Kister polynomial. In thermodynamic properties, the integral excess Gibbs free energy of mixing and the activities of the components of the alloy were investigated using the thermodynamic database of its constituent binary sub-systems. Surface properties, such as surface tension and surface concentrations of components of the alloy were computed using the Butler's model with the aid of determined thermodynamic functions. The excess Gibbs free energy on mixing was found to be negative for the system at all preferred cross-sections and temperatures. However, the negative values of the excess Gibbs free energy of mixing decreased with an increase in the temperatures of the system. The activities of individual components of the system increased, and the surface tension of the system decreased linearly with an increase in temperature. The above-mentioned mixing properties of the alloy computed using GSM, Kohler and Toop model were found to be consistent with each other.

B1-0006

Synthesis, electronic and optical properties of FeVO₄ nanoparticles

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Abstract. Photocatalytic water splitting is a cost effective and environmentally friendly method that helps to solve the ever-increasing global problem for energy demand. As the application section looks practically achievable but finding the stable and suitable photocatalyst material having optimum band gap favoring efficient photon absorption especially visible part of the solar spectrum, band edge positions relative to the water redox potential and high efficiency is quite challenging and hard to achieve. Ferric Vanadate (FeVO₄) is one of the emerging materials with the optimal optical band gap (~2.1 eV). However, the electronic band gap crucially depends on the synthesis parameters used. In this work, to explore the effect of various synthesis approaches and parameters on material property we have used two methods co-precipitation and hydrothermal for the synthesis of FeVO₄ and then calcination was done. The ferric nitrate nonahydrate and ammonium vanadate were used as a precursor material for the synthesis of FeVO₄. The material prepared using these two methods show different results by varying pH values (2, 6, 8, 12). The morphologies of prepared material having different pH values were studied using X-ray diffraction (XRD) and scanning electron microscope (SEM). The UV-Vis characterization was employed to calculate the absorption coefficient of material. Another factor of variation in calculated various results are due to the influence of different phases of material at different temperatures. The sample shows best optical absorption performance at pH 8 while at other pH shows poor absorbance. When the above two methods are compared, the hydrothermal method shows superior results than the co-precipitation method because the sample remained unaffected by the external environment. The FeVO₄ has various applications other than in the field of hydrogen production and evolution, such as CO₂ reduction, removal of organic heavy and organic pollutants.

Study of LuScO₃ perovskite in the cubic phase

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Abstract. In the field of theoretical studies, the first-principles calculations have emerged as a viable method of computing the physical properties of materials. In the present work, we explored the structural, electronic, and mechanical properties of LuScO₃ perovskite oxide using density functional theory (DFT), a first principle method. For this, we have employed Wien2K software based on the full potential linearized augmented plane wave method. LuScO₃ compound has been found to be cubic with space group Pm3m (221). From Birch-Murnaghan fitted curve, we obtained an optimized structure and hence ground state properties like bulk modulus, lattice constant, and derivative of bulk modulus have been calculated. LuScO₃ compound is found to have a direct bandgap of 1.8 eV. The total density of states and partial density of states has also been calculated. The electron density plot reveals that there is covalent bonding between the Sc-O pair and ionic bonding between Lu-Sc & Lu-O pairs. Also, LuScO₃ is found to be brittle in nature as reflected by its elastic property. It could find suitable applications in the solar energy field.

B1-0008

Performance of Double Basin Solar Still Integrated with Evacuated Tubes

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Abstract. To improve the daily productivity of single effect solar still integrated with vacuum tubes; double basin solar still was fabricated as per design specification and installed at the Department of Unconventional Energy Sources and Electrical Engineering, Dr. PDKV, Akola. The performance of the system was evaluated at full load condition for winter and summer season at 3 cm and 4 cm water depth. At 3 cm water depth evaporation rate was higher and hence distillate yield was found more of about 11 liters in winter and 14 liters in summer. The energy efficiency is the ratio of amount of thermal energy utilized to get amount of distilled water to incident solar energy within a given time. The energy efficiency found in the range of 28.62 to 30.59 per cent and 25 to 26.78 per cent at 3 and 4 cm water depth, respectively in winter and 37.92 to 38.89 per cent and 33.95 to 35.00 at 3 and 4 cm water depth, respectively in summer.

A study of Thermal Parameters by employing TGA and DSC of Copper Metal Complexes K R Patel¹, K P Patel² and V D Patel³

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Abstract. The nature and content of Metal and Ligand have a significant impact on the behavior and properties of Metal Complexes. Metal Cu(II) with Ligands, 2-Mapthye Amine(2-MA), P-Dimethyle Amine Benzaldehyde (PDAB) and Di(2-pyridyl)amide (DPA) were used to synthesized Metal Complexes. Author synthesized three complex named ML1L2, ML2L3 and ML3L1 for scientific investigation. In the current paper, thermal behavior using TGA of all the complexes were studied and discussed in details. The derivatives data were created to analyze the thermogram properly. The thermodynamics parameters were also determined with Broido method. Parameters such as Activation Energy Enthalpy, Entropy and Gibbs energy were computed from the TGA data using Broido method. The dynamic temperature aspect has been considered eventually and the results were presented in respective section. The DSC measurements curve illustrates heat flow with rising temperature. Specific heat (Cp & Cv), Heat, Heat Capacity and thermal diffusivities of complexes were measured form the analytical data. The investigation peak and region corresponding to enthalpy involved in the process has been identified in schematic DSC curve. Present investigation deals with measurement of the various thermal parameters of complexes besides some other thermal event measurement briefly discussed at room temperature to decomposition temperature.

B1-0010

Nanotechnology In Engineering

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Abstract. In recent years, nanotechnology has been explored with great interest due to its usage in various fields like physics, chemistry, material science, medical and engineering. The nanotechnology is emerged as major research area for researchers. The nanotechnology fabricates, characterizes and handles the materials at nanoscale. Nanotechnology applications commonly include industrial, medical and energy applications. Reducing the particle size to a nano-scale enhances several properties of the materials for example, durability, strength, ductility, density of the construction materials, buoyancy, ruggedness, storage efficiency of Li batteries etc.

Hydrogen Storage Potential and Properties of Yttrium Doped C₂₀ Fullerene: Insight from Density Functional Theory

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Abstract. Hydrogen storage for sustainable energy fuel with high capacity in ambient conditions is a major challenge in recent times¹. We investigated the molecular hydrogen adsorption/desorption potential and properties of yttrium (Y) doped C₂₀ fullerene using the dispersion corrected density functional theory calculation. Four Y metals are functionalized on the bridge position of C₂₀ and are bonded with a binding energy of 2.1 eV per Y atom through covalent interaction. The sequential adsorption of hydrogen molecules Y doped C20 reveals that each Y atom can hold up to five H2 molecules via Kubas mechanism. The average adsorption energy decreases with successive addition of H_2 molecules with binding energy lying in the range of 0.25 eV - 0.28 eV/ H_2 . This range of adsorption energy infers the physisorption of H₂ with the sorption center, and the fact is also supported by the distance of H₂ molecules from the sorption center. The system can have a maximum gravimetric density of 6.34 wt%, that faily above the US-DOE target. Stabilities of the studied systems were confirmed by various reactivity parameters such as hardness (η), electrophilicity (ω), electronegativity (γ). Calculated reactive parameters revealed the stability of the hydrogenated system by following the maximum hardness and minimum electrophilicity principle. To quantify the number of hydrogen molecules available for use at diffrenet thermodynamic conditions, the occupation number of H₂ was calculated at a wide range of temperature and pressure. Consistent with criteria set by the US-DOE, Y doped C₂₀ can be used as promising hydrogen storage materials.

B1-0012

Structural And Electrical Properties Of Low Energy Ion Beam Kr Irradiated Bi/Se Bilayer Anil K Das^{1,a)}, Manju Bala^{2,b)}, Vikram Singh^{1,c)}, D.K. Avasthi^{3,d)}, K. Asokan^{3,e)}, Prabhakar Singh^{1,f)}, S.A. Khan^{4,g)}

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Abstract. In the present work Bi (~50nm)/Se (~50nm) thin films were deposited successively on the Silicon substrate by e-beam evaporation method under 2×10-5 mbar pressure at room temperature. Ion beam processing is one of the distinctive approaches to create thin films, and it has recently been employed to create thermoelectric thin films. It was demonstrated that these thermoelectric films made with an ion beam were nanostructured and had a higher Seebeck coefficient. Applications for binary Bi2Se3 thin films, which are part of group V-VI, include photoconductivity, photosensitivity, and thermoelectric power. It is a semiconductor with a small band gap. It has drawn a lot of interest because of its alluring thermoelectric and Hall effect uses. The Bi/Se bilayers were irradiated with ion beams of 350 KeV Kr+1. The samples were then characterised by XRD, SEM and Rutherford backscattering spectrometry (RBS). Since the irradiated sample offered very high resistance its electrical measurements were not carried out. Electrical measurements like Hall effect, Seebeck coefficient and resistivity were carried out for pristine sample and pristine structural results were compared with irradiated sample.

Thermal Properties of V₃SI

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Abstract. Using the *ab-initio* FP-LAPW technique, the structural and thermal characteristics of V_3Si are investigated. The equilibrium structural parameters and the formation enthalpy obtained are in good agreement with the results of the existing experimental and theoretical data. To determine the internal energy, Helmholtz free energy, entropy, heat capacity at constant volume and pressure, Grüneisen parameter, thermal expansion coefficient and Debye temperature of V_3Si , the *ab-initio* total energy calculations are linked with the second-generation software Gibbs2. It employs the Debye Slater and Debye Grüneisen models. The existing experimental and theoretical data are in accord with all of the current findings.

B1-0014

Study of negative permittivity behavior Sr₇Mn₄O₁₅-SrO nanocomposite

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Abstract. Negative permittivity has been researched extensively in a wide range of metamaterials and composites. Using a solid-state ceramic route, a composite of Sr₇Mn₄O₁₅ - SrO has been produced. At all measured frequencies (10 Hz-2MHz) a change in signof permittivity from positive to negative is found above a specific temperature (T_c). Experimental data of real part of permittivity was fitted to Drude-Lorentz oscillator model. The cause of negative permittivity was found to be plasma oscillations of thermally excited free carriers. High temperature plasma plasmonic activity of synthesized composite make it promising metamaterial for electromagnetic devices working in the radio frequency (10 Hz -2MHz) range

Study of Grüneisen Parameter and Debye temperature for hcp-iron under High Pressure

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Abstract. We have derived the expression Debye temperature for hcp-iron using the volume dependence Grüneisen parameter $\gamma(V) = \gamma_0 \left[1 + a \left\{ \left(\frac{V}{V_0} \right)^b - 1 \right\} \right]$, where a and b are volume independent adjustable parameters. Using the formulation of γ , we have determined the expressions for the second-order Grüneisen parameter, Debye temperature and the shear velocity for hcp-iron. However, even though the Grüneisen parameter and the equation of state (EOS) are directly connected, it is often the case that individual forms of γ and the EOS can selected independently. Therefore, the equation of state, Bulk modulus and its first derivative of bulk modulus have been also determined for hcp-iron using the Eulerian finite theory which is based on n-th power of edge length by compression recently reported by Singh et al. We have calculated the Grüneisen parameter, second-order Grüneisen parameter, Debye temperature and the shear velocity for hcp-iron in order to test the applicability of the present formulation. The obtained results are very close and compatible with experimental data.

B1-0016

Study of negative permittivity behavior Sr₇Mn₄O₁₅-SrO nanocomposite

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Abstract. Negative permittivity has been researched extensively in a wide range of metamaterials and composites. Using a solid-state ceramic route, a composite of Sr₇Mn₄O₁₅ - SrO has been produced. At all measured frequencies (10 Hz-2MHz) a change in signof permittivity from positive to negative is found above a specific temperature (T_c). Experimental data of real part of permittivity wasfitted to Drude-Lorentz oscillator model. The cause of negative permittivity was found to be plasma oscillations of thermally excited free carriers. High temperature plasma plasmonic activity of synthesized composite make it promising metamaterial for electromagnetic devices working in the radio frequency (10 Hz -2MHz) range.

Iron Oxide-Molybdenum Di-sulfide Composite for Enhanced Hydrogen Evolution Reaction Activity

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Abstract. In pursuance to achieve green future, electrochemical water splitting can be potential technology to address the global need to replace the polluting fossil fuels. In order to search non precious and non noble metal based electrocatalysts we successfully synthesized Iron Oxide-Molybdenum Di-sulfide (Fe₂O₃-MoS₂) via two step facile synthesis route. Fe₂O₃-MoS₂ exhibits significant lower overpotential, 202 mV, to drive 10 mA cm⁻² current density and the value is superior to the individual components, Fe₂O₃ and MoS₂. The low charge transfer resistance 13.9 Ω signifies the faster charge transfer at the electrolyte-catalyst-interface facilitating HER performance. The sample also shows good stability and durability under the acidic medium. The higher value (10.3 mFcm⁻²) of electrocatalytic double layer capacitance C_{dl} corresponding to Fe₂O₃-MoS₂ composite further confirms the ample availability of electrocatalytic active sites. The study establishes a successful TMO –TMD composite as a potential candidate for HER performance in acidic medium and opens up new opportunities for finding proper electrocatalyst towards 'green hydrogen'.

B1-0018

Structural and Electrical Properties of Low Energy Ion Beam Kr Irradiated Bi/Se Bilayer Anil K Das 1,a , Manju Bala 2,b , Vikram Singh 1,c , D.K. Avasthi 3,d , K. Asokan 3,e , Prabhakar Singh 1,f , S.A. Khan 4,g

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Abstract. In the present work Bi (~50nm)/Se (~50nm) thin films were deposited successively on the Silicon substrate by e-beam evaporation method under 2×10⁻⁵ mbar pressure at room temperature. The Bi/Se bilayers were irradiated with ion beams of 350 KeV Kr⁺¹. Ion beam processing is one of the distinctive approaches to create thin films and it has recently been employed to create thermoelectric thin films. It was demonstrated that these thermoelectric films made with an ion beam were nanostructured and had a higher Seebeck coefficient. Applications for binary Bi₂Se₃ thin films, which are part of group V-VI, include photoconductivity, photosensitivity, and thermoelectric power. It is a semiconductor with a small band gap. It has drawn a lot of interest because of its alluring thermoelectric and Hall effect uses. The samples were then characterised by XRD, SEM and Rutherford backscattering spectrometry (RBS). Since the irradiated sample offered very high resistance its electrical measurements were not carried out. Electrical measurements like Hall effect, Seebeck coefficient and resistivity were carried out for pristine sample and pristine structural results were compared with irradiated sample.

Comparison of the Crystal Structures of Three Compounds with a Phenoxy Acetohydrazide Nucleus

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Abstract. Three compounds containing phenoxy acetohydrazide and their crystal structures were compared for derivatives of 2-methyl-phenoxy)acetohydrazide,2-(4-Methoxyphenoxy)acetohydrazide, and 2-(4-Methylphenoxy)acetohydrazide. Structures 1 and 3 crystallised in the monoclinic crystal system with fedorov groups P2/n and P21/c, whereas Structure 2 did so in the orthorhombic crystal system with fedorov group $P2_12_12_1$. With the use of single crystal X-ray diffraction data taken at room temperature and full-matrix least-squares refinement techniques, the crystal structures of all three molecules were determined. The Reliable Index of the aforementioned compounds was discovered to be 0.0377 and 0.030 for derivatives 1 and 2, and 0.067 for compound 3.

B1-0020

Enhance Photon Upconversion Emission in with Er₂O₃ and AgNO₃-doped Tungsten Tellurite Glasses

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Abstract. There has been research on the frequency upconversion in Er³⁺ doped tungstate-tellurite doped glass with silver nanoparticles (NPs). By using the melt quenching procedure with a modest number of Ag nanoparticles, tellurite-based glasses have been created (Ag-NPs). The optical excitation occurs at 980 nm in resonance with the transition of Er³⁺ ions in the glass system from ⁴I_{15/2} to ⁴I_{11/2}. As Er³⁺ ions transitioned, emission bands with centres at 535nm, 550nm, and 664nm were seen. This TWNEA with Ag NPs glass sample analysis concerned the assessment of the intensity of the green and red colours. According to the results, it is possible to use glasses doped with rare earth elements and silver to explore the possibilities of multiphoton microscopy.

Detection of Carbon Monoxide in Automobile Vehicles

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Abstract. Carbon monoxide is one of the most dangerous gas affecting the people travelling in the automobile vehicles with the permissible exposure level of 35ppm. In order to reduce the mortality rate due to Carbon monoxide poisoning, we could implement a system to detect the increase in the intensity level of carbon monoxide inside the cars cabin with the help of carbon monoxide gas sensor. The circuit is constructed using Raspberry Pi and MQ-7 gas sensor. If the Carbon monoxide level reaches 400 parts per million and above, the system could automatically switch off the air conditioner and turn on the fan to control the intensity level of carbon monoxide gas inside the cabin to the permissible exposure level.

B1-0022

Anionic Effect on Electrical Transport Properties of [(1-x) Succinonitrile-xPoly(Ethylene Oxide)]-LiX (X = TFSI or Triflate)-Co(bpy)₃(TFSI)₂-Co(bpy)₃(TFSI)₃ Solid Electrolytes
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Abstract. A redox mediator (electrolyte) is an integral part of the dye-sensitized solar cell for the regeneration of the dye molecules. The electrolyte in solid nature helps to keep the device lightweight, affordable, and safer. This paper has presented the electrical transport properties of [(1-x)succinonitrile-x poly(ethylene oxide)]- LiX- Co(bpy)₃(TFSI)₂- Co(bpy)₃(TFSI)₃ solid electrolytes, where x is 0, 0.5, and 1 in weight fraction. The anion, X is either bis(trifluoromethyl) sulfonylimide (TFSI; ionic size 0.7 nm) or trifluoromethanesulfonic acid (triflate; ionic size 0.44 nm). The electrolytes with TFSI⁻ exhibited electrical conductivity ($\sigma_{25^{\circ}\text{C}}$) of $2.1 \times 10^{-3} \text{ S cm}^{-1}$ for $x = 0, 7.2 \times 10^{-3}$ ⁴ S cm⁻¹ for x = 0.5, and 9.7×10^{-7} S cm⁻¹ for x = 1. The triflate ions-based electrolytes had lower $\sigma_{25^{\circ}\text{C}}$ values, 1.5×10^{-3} for x = 0, 3.1×10^{-4} for x = 0.5, and 6.3×10^{-7} S cm⁻¹ for x = 1. This is due to a larger size of TFSI ions, which has a lower value of lattice energy with delocalized electrons, resulting in highly dissociable salt in the solvent with a less anionic contribution to the total conductivity. The $\log \sigma$ -T⁻¹ study exhibited Arrhenius-type behavior for electrolytes with x = 0 and 1, and Vogel-Tamman-Fulcher-type behavior for the blend-based electrolytes (x = 0.5). The anionic effect is explained using various characterization techniques, such as x-ray diffractometry, Fourier transforms infrared spectroscopy, UV-visible spectrophotometry, polarized optical microscopy, scanning electron microscopy, differential scanning calorimetry, and thermogravimetric analysis. The results were also compared with those of acetonitrile–LiX–Co(bpy)₃(TFSI)₂–Co(bpy)₃(TFSI)₃ liquid electrolytes. Only the electrolytes with x = 0.5 offered thermal stability up to 125 °C with transparency in UV-A, visible, and near-infrared regions, making them suitable for the device application.

A Computational Study Of Pure 60.6 And Fluorinated 60.6 Liquid Crystalline Molecule

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Abstract. Density functional theory (DFT) simulations are used in this study to examine the structural properties and vibrational behavior of pure 6O.6 and fluorinated 6O.6 liquid crystalline compounds. We investigate the molecular interactions of the molecule by investigating its optimized molecular structure and its infrared (IR) spectra. Identification of significant functional groups and their dynamic behaviors are made with the help of the vibrational frequencies obtained through DFT calculations, which act as instructive fingerprints of the molecular composition. Our investigation focuses particularly on the strong peaks associated with the C-H stretching, C=N stretching, and CC stretching modes. Furthermore, changes in vibrational peaks provide insight into structural modifications. This study advances knowledge of liquid crystalline materials by thoroughly examining the structural and vibrational properties of the compound, and it opens a path for further investigations into optoelectronic applications and molecular dynamics.

B1-0025

Sr₃(PO₄)₂:Sm³⁺- A Promising Yellow-Emitting Phosphor Candidate for Luminescence Boltzmann Thermometers.

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Abstract. The present study explores the luminescent and thermometric characteristics of Sm^{3+} doped $Sr_3(PO_4)_2$ [SPO] phosphors prepared by an economical combustion synthesis technique. The XRD study confirms the single-phase hexagonal crystal structures of the phosphors. The photoluminescence (PL) spectra demonstrate a characteristic yellow emission ascribed to the $^4G_{5/2}$ to $^6H_{7/2}$ transition of Sm^{3+} ion when the phosphor is excited with 400 nm UV light. The emission is characterized by CIE chromaticity coordinates located at (0.56, 0.44). Temperature-dependent photoluminescence (TDPL) properties of SPO: Sm^{3+} samples are carefully studied by the Luminescence Intensity Ratio (LIR) technique. The results illustrate the impressive sensitivity of the sample, with a peak absolute sensitivity of 0.0065 % K^{-1} at 761 K and a relative sensitivity of 1.70 % K^{-1} at 304 K. Hence, Sm^{3+} doped SPO phosphors hold significant promise for applications in optical thermometry.

Comprehensive Structural and Luminescence Investigation of Yellow-White Emitting Ca₂B₂O₅:Dy³⁺ Phosphors for UV-based White LED Applications

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Abstract. In this work, undoped and a series of $Ca_2B_2O_5$:Dy³⁺ phosphors have been synthesized via low-cost consuming, self-propagating solution combustion method (SCS). The X-ray diffraction (XRD) and Fourier-transform infrared (FTIR) spectra confirmed the creation of a single-phase monoclinic structure and the presence of BO_3 and BO_4 groups in both synthesized samples. Room temperature photoluminescence (PL) excitation spectra for both samples exhibited strong absorption bands in the near ultraviolet (UV) region, while the emission spectra displayed two prominent emission bands around 484 nm (blue) and 577 nm (yellow), corresponding to the ${}^4F_{9/2} \rightarrow {}^6H_{15/2}$ and ${}^4F_{9/2} \rightarrow {}^6H_{13/2}$ electronic transitions, respectively. Photometric measurements revealed that the CIE (Commission International de'Eclairage) coordinates lies in the yellowish-white region of the CIE color gamut with average lifespan of 0.03 ms. Thermogravimetric Analysis (TGA) indicates that the synthesized samples have good thermal stability. All results findings indicate that the yellowish-white emitting Dy³⁺ activated $Ca_2B_2O_5$ phosphors, providing enhanced properties suitable for White light emitting diodes (W-LED) applications and display devices.

B1-0027

Interfacial Modifications in ZnO/PEDOT:PSS Heterojunction by CuS Based Composite Matrix

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Abstract. The study reports the synthesis of CuS-PVP nanocomposite matrix by simple aqueous solution processing method and used to prepare a ZnO/CuS-PVP/PEDOT:PSS sandwich type heterostructure device. The ZnO was grown on the ITO flexible PET substrate by low-cost hydrothermal method and further the CuS-PVP was spin coated over them. The XRD reveals the hexagonal wurtzite structure of the ZnO growth and the decoration of CuS-PVP was further confirmed by the presence of the additional diffraction planes corresponding to the hexagonal covellite phase of the CuS. The broad emission peak of ZnO at 390 nm in the PL spectra suffers a significant decrease in intensity after CuS-PVP loading in ZnO/CuS-PVP sample. The conjugation of CuS with PVP was further justified by the FTIR analysis. It is found that the CuS-PVP insertion layer in the ZnO/PEDOT:PSS n-p heterojunction plays a major role in the performance enhancement as the rectification ratio of the samples at ±2V increases 17 times after the addition of the CuS-PVP layer. The transient photoresponse (J-t) of samples with and without CuS-PVP layer at 0V bias were measured under the illumination intensity of the 100mW/cm² which were analyzed by switching light on and off in a constant time interval. For several cycles, the devices shows repeatable trend which corroborates the stable photoresponse behaviour. The change in the photocurrent J_{light}- J_{dark} for samples with and without CuS-PVP insertion layer was found to be 1.76 and 0.795 μA/cm² respectively. This study provides a novel approach for controlling the charge carrier dynamics at ZnO/PEDOT:PSS interface and may find use in self-powered photo-detection, highly efficient solar cells, advanced sensors and so on.

Ni-MOF Derived Bimetallic Nanoalloy: An Excellent UOR Electrocatalyst

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Abstract. Urea Oxidation Reaction (UOR) has the potential to deal with two major concerns of the modern world, one is polluted wastewater and the other one is fossil fuel dependency, both contributing to global hazards. By efficiently splitting urea-rich wastewater via UOR, green Hydrogen energy can be generated with appropriate electrocatalysts, killing two birds with one stone. Herein, an efficient UOR active catalyst, Ni-C/MoO₂ has been successfully synthesized by integrating Mo element with a Ni-MOF in elevated temperature within an inert atmosphere. The as-prepared catalyst exhibits a much higher UOR activity in 1M KOH solution mixed with 0.5M Urea, needing a potential of only 1.45 V to achieve a current density of 10mAcm⁻², whereas without urea it requires 1.6 V to gain a similar current density. A very low Tafel slope of only 32 mV dec⁻¹ indicates that the reaction rate drastically improves in the presence of urea compared to 122 mV dec⁻¹ without it. The superior catalytic activity is explained by the enriched electronic structure of Nickel active sites by the introduction of Molybdenum dioxide, diminishing the charge transfer resistance and thereby accelerating the reaction rate. This work provides insights on the importance of UOR with properly designed electrocatalysts as a much-needed substitute for the energy-taxing OER for a greener but more importantly economical hydrogen society of the future.

B1-0029

Temperature Dependent of Elastic Modulus for Porous Superconducting Material YBCO Hamdi Farah 1,a)

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Abstract. Elastic constants help us understand the behavior of the material, spatially relative to the superconductor material; these constants play additional key roles. We emphasize that the variation of temperature effect on the elastic constants and ultrasonic wave's velocity of a superconducting material for non porous and porous state. Besides, temperature and porosity can be considered independent variables within a suitable temperature range.

In this context, this work studies the effect of temperature by simulating the elastic properties of the Y1Ba2Cu3O7-x (YBCO) superconducting materials in the nonporous and porous state. The acoustic signal, V(z), received from the acoustic microscopy is used in the study by analyzing it through the simulation of reflection coefficient. From the analysis of V(z) by transformed Fourier (FFT), the estimated evolution of Young (E) Bulk (K) and Shear (G) modulus depending on the temperature for different porosity rates were also determined. Finally, the efficacy of the proposed methodology has been established with experimental data and the models obtained on porous and nonporous YBCO superconducting materials from previously published studies.

Exploring the Physics and Analysis of Desiccation in Soil: Insights from Euler Number, Fractal Dimension, and Water-Mass Ratio

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Abstract. Soil desiccation cracking is a usual natural phenomenon which is due to changing water-mass ratio in the soil body. The objective of this study is to establish a relationship between the water-mass ratio and the desiccation crack formation in the soil using the fractal dimension and Euler number, by examining the weight loss or water-mass ratio and crack formation over time due to desiccation. The soil used in the study had the maximum water holding capacity of 39.50% with a texture distribution of 30.32% Clay, 19.97% Silt, and sand 49.70%. Notably, the fractal dimension and the Euler number of the desiccation crack changes depending on the thickness of the sample. The study contributes to the broader understanding of how the fractal dimension and Euler number are affected by the thickness and water-mass ratio.

B1-0031

Transition Energy For a Polar Quantum Disc with Conical Disclination in Parabolic Confining Electric Potential

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Abstract. Transition energy of electron for a polar quantum disc with conical disclination is investigated theoretically. For charge carrier confinement, we consider the infinite square well potential (IPSW), and parabolic potential (PP). The disclination in the system is characterized by the kink parameter κ . The energy levels of the system were calculated using the Schrödinger equation with the effective mass approximation. Our study reveals that the transition energy decreases as the kink parameter κ increases.

Fabrication of Metal Organic Framework/Graphene Oxide Nanocomposites: Synergy of Photocatalysis and Adsorption for the Removal of Aquatic Pollutants

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Abstract. Metal-organic framework (UiO-66) and its composite with GO were successfully synthesized by a facile hydrothermal method. X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray (EDAX), and transmission electron microscopy (TEM) were used to characterize the synthesized material. Rhodamine-B (RhB) was chosen as the model water contaminant for this paper. Studies on adsorption were done in the dark, and those on photocatalysis were done outside in the daylight. In comparison to pure MOF, the MOF/GO composite has enhanced adsorption and photocatalytic activity. RhB is eliminated by 99% in a very short time through the combined action of adsorption and photocatalysis of the composite. The surface, thermal stability, and mechanical strength of the metal-organic framework are all boosted by introduction of graphene oxide. The MOF/GO composite fabricated in this way would serve as an excellent photocatalyst for the gradual removal of aquatic pollutants that would be affordable, effective, and ecological

B1-0034

Quantum Transport Properties of Monolayer MoS2, WS2, and Black Phosphorus: A Comparative Study

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Abstract. A comparative study of the performance analysis of dual-gate ballistic monolayer Molybdenum disulfide (MoS₂), tungsten disulfide (WS₂), and black phosphorus (BP) field-effect transistors (FETs) is presented. A thorough investigation of output and transfer characteristics infers that WS₂ FET exhibits better performance as compared to MoS₂ and BP. Furthermore, among all three FETs (MoS₂, WS₂, and BP), the WS₂ based FET has a higher carrier velocity. However, variation of gate capacitance (C_G) with gate voltage (V_G) reflects a very good electrostatic gate control of MoS₂ FET due to higher surface charge accumulation. Except for C_G , the overall performance of WS₂ based FET is better than MoS₂ and BP.

Optical Characterization Of Na₂ZrO₃:Dy³⁺ Phosphor Synthesized By Combustion Route

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Abstract. The present study involves the synthesis of a phosphor material, specifically Dy³⁺ doped Na₂ZrO₃, by a solution combustion synthesis method utilizing urea as the fuel source. The synthesized materials undergo characterization using X-ray diffraction (XRD), UV-Vis spectroscopy, and photoluminescence (PL) spectroscopy. The XRD results confirm the synthesis of single-phase phosphor. Using the Scherrer formula the crystallite size is calculated and found to be 24 nm. According to photoluminescence (PL) results, it has been observed that when subjected to stimulation at a wavelength of 351 nm, the phosphor material demonstrates a prominent emission band with a peak centered at 585 nm. The optimal concentration of the dopant is observed at a concentration of 3 mol.%. The CIE color coordinates (0.37, 0.41) indicate that the emission color falls within the yellow-whitish region of the color gamut. This particular color has an associated color temperature of 3073 K. The optical direct bandgap, as determined through the use of diffuse reflectance spectroscopy (DRS), is seen to be 5.27 eV for the sample that exhibits optimal characteristics. The findings of this study indicate that the synthesized phosphor has the potential for future utilization as a white light-emitting diode (WLED) in solid-state lighting applications. This phosphor demonstrates promising performance when stimulated by a near-ultraviolet (n-UV) source with a wavelength of 351 nm.

B1-0036

Electronic, Optical and Thermoelectric Properties of Halide Double Perovskite Cs₂CuSbX₆ (X = Cl, Br, I)

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Abstract. The exploration of novel materials with advanced optical and thermoelectric characteristics has gained significant attention due to their potential for technological applications. Our work delves into the in-depth study of new halide double perovskites Cs_2CuSbX_6 (X = Cl, Br, I), a class of materials that has recently emerged as promising candidates for various optoelectronic and thermoelectric applications using DFT and semi-classical Boltzmann transport theory. The optical properties of Cs_2CuSbX_6 , including absorption, reflectivity, and dielectric function etc., are comprehensively investigated, shedding light on their potential for efficient light-harvesting and emission in optoelectronic devices. Furthermore, the thermoelectric properties of Cs_2CuSbX_6 are systematically examined, focusing on the electronic band structure, Seebeck coefficient, thermal conductivity, and the efficiency. The intricate interplay between the optical and thermoelectric characteristics is explored to elucidate the design principles for optimizing these properties for specific applications. Through a critical review, our work provides valuable insights into the fundamental mechanisms that govern the optical and thermoelectric performances of halide double perovskites Cs_2CuSbX_6 (X = Cl, Br, I), ultimately contributing to the development of next-generation energy-efficient devices and systems.

Critical Review on Functional Materials for Sustainable Energy

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Abstract. Research on sustainable energy is assisted by a variety of structural and functional materials that have advanced during the past ten years. Functional materials are very effective in the physical processes, whereas structural materials provide the functionality of load support. With the innovative development in the material's electrical, magnetic, optical, or chemical capabilities, multifunctional structures and gadgets are used in a wide variety of applications. Graphene (2D material) to create nanocomposite materials is mostly used functional material, to improve the conductivity and reproducibility of the cathode material. Structural materials are having their limitations hence dense anode materials are used to avoiding such issues like converting, alloy and dealloying process. Ionic liquids for electrochemical energy storages are still under research, although the Lithium-ion batteries (LiBs) are providing a considerable level of power storage and power potential. This chapter examines the role and technology of nanomaterials from its inception to prospective developments in the future for sustainable energy.

B1-0038

Reinforcements and Processing of Aluminium Matrix Composites for automotive and aerospace applications

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Abstract. Aluminium matrix composites combine the strengths of aluminum and other materials to create materials with tailor-made properties. These materials are engineered to excel in specific applications where the properties of aluminum alone would be insufficient or inadequate. Reinforcing aluminum with other materials can lead to composites with improved properties. This article critically reviews ceramic reinforcements, bio-reinforcements and other natural reinforcements to improve tensile strength, improved thermal expansion behavior, enhanced wear resistance, and increased fatigue resistance compared to pure aluminum. It further deals with the review of manufacturing processes like powder metallurgy, in-situ synthesis, solid state welding and casting. The choice of manufacturing method depends on the type of reinforcement and the desired properties of the composite.

Ab-initio Investigation of Elastic Properties of Monoclinic ZnAs₂ Crystal

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Abstract. Elastic properties of monoclinic ZnAs₂ crystal are studied under the PBEsol scheme using the CRYSTAL Program. Independent elastic stiffness coefficients have been computed. Various elastic properties, such as shear modulus, bulk modulus, Young's modulus and Poisson's ratio have been analyzed. The directional dependence of the computed Young's modulus and linear compressibility is studied using ELATE software. Our investigation reveals the finite elastic anisotropy of the monoclinic ZnAs₂ crystal.

B1-0040

Pd-doped SWCNT as Nanobiosensor for Phenylalanine Hydrolase

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Abstract. We examined Pd-doped single walled carbon nanotube (SWCNT) as a bio-nanosensor for the detection of phenylalanine amino acid (Phe) using DFT simulations. Three distinct phenylalanine adsorption sites around the Pd atom of nanotube, each possessed unique properties and adsorption, after thoroughly being optimized. In order to explore the sequence of bonding strength in complexes and get a thorough knowledge of their interactions with Phe-Pd/SWCNT, chemical properties, NBO, and QTAIM analyses have been conducted. Chemical potential and hardness were computed using DFT/B3LYP with the 6-31G* and the DGDZVP for the Pd atom as the parameters representing chemical reactivity and stability. The results we obtained show that Pd/SWCNTs can function as a bionanosensor due to their high binding energy and considerable transmission of charge caused by the adsorption of phenylalanine amino acid.

Pd-doped SWCNT as Nanobiosensor for Phenylalanine Hydrolase

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Abstract. We examined Pd-doped single walled carbon nanotube (SWCNT) as a bio-nanosensor for the detection of phenylalanine amino acid (Phe) using DFT simulations. Three distinct phenylalanine adsorption sites around the Pd atom of nanotube, each possessed unique properties and adsorption, after thoroughly being optimized. In order to explore the sequence of bonding strength in complexes and get a thorough knowledge of their interactions with Phe-Pd/SWCNT, chemical properties, NBO, and QTAIM analyses have been conducted. Chemical potential and hardness were computed using DFT/B3LYP with the 6-31G* and the DGDZVP for the Pd atom as the parameters representing chemical reactivity and stability. The results we obtained show that Pd/SWCNTs can function as a bionanosensor due to their high binding energy and considerable transmission of charge caused by the adsorption of phenylalanine amino acid.

B1-0042

FT-IR and XRD Study on Polyvinyl butyral and Poly (vinylidenefuoride-co-Hexafluoropropylene) Blends

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Abstract. The commercial Polyvinyl butyral (PVB) and Poly (vinylidenefuoride-co-Hexafluoropropylene) (PVDF-HFP) used in the present investigation were prepared by the solution cast technique. Blend samples of wt% compositions PVB: PVDF-HFP:: 95:05; 90:10; 85:15 and 80:20 were prepared. The prepared films were characterized by FTIR and XRD techniques for structural and morphological studies. FTIR and XRD analysis confirms the molecular interaction between the two polymers and also the dominating presence of α -phase PVDF-HFP in blends. Studies also reveal that the crystallinity occurs in blend samples with increase of PVDF-HFP wt%. Different characterization in present investigation indicates that prepared blends are compatible in selected composition range.

Structural, Electronic and Vibrational Properties of PdS Monolayer: A First Principle Approach

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Abstract. Motivated by the extravagant optoelectronic and thermoelectric properties of recently reported potential transition metal monochalcogenides, we proposed a new palladium based monolayer PdS. As the monolayer is new, so it is necessary to validate its stability. Positive vibrational mode in the phonon dispersion curve and negative formation energy confirms the dynamical and chemical stability of the monolayer respectively. Lattice dynamics of the monolayer are investigated by using density perturbation theory. Electronic band structure of the monolayer has been studied by employing the PBE functional. All the results indicate the potential application of the monolayer in emerging fields.

B1-0044

Thermal and electrical properties of rare earth based chalcogenide compounds R_2X_3 (R=Dy or Tb and X=S or Se)

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Abstract. Electronic and thermal properties of rare-earth chalcogenide compounds R_2X_3 (R=Dy/Tb and X=S/Se) are investigated using Density Functional Theory and the Boltzmann Transport Equation. The effective mass, deformation potential and elastic constants are calculated. The rare-earth chalcogenide compounds are dynamically stable. The lattice thermal conductivity for these compounds is calculated using slack model. The lowest value of k_1 4.5W/mK is obtained for Tb_2Se_3 This low thermal conductivity of these compounds can have several applications in various fields like thermoelectric, thermal insulation and phononics.

TL and OSL Study Of Sm Doped NaMgF3 Phosphor Irradiated With Gamma Rays

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Abstract. The measurement of the ionizing radiation using highly sensitive TL/OSL based radiation dosimeters with great precision and accuracy is increasing worldwide. In medical dosimetry, it is important to monitor the dose delivered to the patients within permitted limits to ensure the nondestruction of healthy tissues. NaMgF₃ is one of the materials with great interest due to its interesting properties such as tissue equivalency, non-toxicity, low hygroscopicity, high thermal stability, wide band gap etc. When doped with certain amount of rare earth ions, its TL and OSL properties is enhanced due to the substitution of RE²⁺/RE⁴⁺ ions for the Na⁺ site and require charge compensation. In this work, we have attempted to prepare the NaMgF₃ phosphor doped with Sm and investigated its TL and OSL properties. The NaMgF₃ doped with Sm has been prepared using solid state diffusion method. The phosphor has been prepared using three different concentrations of Sm i.e., 0.1, 0.2 and 0.5mol%. TL glow curves were recorded from Harshaw O TLD reader model 3500 at heating rate of 5°C/sec. TL and OSL signal response are investigated after irradiation with a gamma dose of 15 Gy. The XRD pattern confirm the formation of the phosphor. The photoluminescence (PL) emission spectra measured for different concentration of Sm (0.1- 0.5mol %) with excitation wavelength of 404nm show the characteristics peaks of Sm³⁺. TL glow curve of the optimized NaMgF₃: Sm (0.2mol %) phosphor has shown a simple glow curve with main peak at 118°C and low intense peaks at 288°C and 365°C. At higher concentration of Sm (0.5mol%), an addition shoulder appeared at 160°C. The nature of the energy traps in Sm doped samples has been analyzed through glow curve deconvolution. A significant OSL signal is also observed at optimized concentration of Sm.

B1-0046

Influence Of Sm Doping On TL Of LiF Crystals grown by EFG technique

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Abstract. Lithium Fluoride (LiF) based thermoluminescence (TL) dosimeters are potential materials for the measurement of the radiation absorbed dose due to its advantages like tissue-equivalence, high sensitivity, energy independence and dose linearity. The incorporation of rare earth (RE) ions as a dopant material show strong influence on the TL properties of the phosphor due to their characteristic's luminescence. In this work, LiF crystals doped with Samarium (Sm) were grown in crystalline form using Edge defined film fed growth (EFG) technique using graphite crucible and stainless-steel die under argon gas atmosphere. The concentration of Sm dopant used was 0.02, 0.05 and 0.1 wt%. XRD pattern confirmed the formation of the LiF: Sm phosphor. TL measurements were made on as grown and annealed crystals after irradiated with a gamma dose (source Co⁶⁰) of 15 Gy. The annealing was done at 400°C for 1 hr and 80°C for 24hr in air. TL glow curve structure of EFG grown LiF: Sm crystal consists of high intense main TL peak at 135°C along with low intense peaks around 200°C and 275°C. TL intensity of LiF: Sm in annealed crystals increased significantly (~10 times) in comparison to as grown crystals. The influence and advantage of Sm ion in enhancing the TL intensity of undoped LiF were discussed. Whereas it is quite difficult to dope the RE ion in host lattice of LiF with other preparation method, LiF: Sm crystal grown using EFG technique showed good incorporation. The kinetic parameters of LiF: Sm phosphor TL glow peaks have been analyzed by Computerized Glow Curve Deconvolution (CGCD) method. Doping with Sm ion has enhanced the TL intensity of undoped LiF due to the increase number of electrons/hole traps inside the material during irradiation which might be useful for dosimetry application.

Effect of Mn- doping on Structural and morphological properties of nanostructured Bi₂Te₃ for thermoelectric applications

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Abstract- Nanostructured Bi₂Te₃ compounds have been synthesized by solvothermal method for thermoelectric applications. XRD results confirmed that synthesized materials have rhombohedral crystal structure with space group of R-3m. FESEM results revealed that synthesized materials have hexagonal plate like morphology. EDS was performed to obtain chemical composition. Mn doping in nanostructured Bi₂Te₃ introduced the mass fluctuation and large density of interfaces which further can decrease the lattice thermal conductivity. Seebeck coefficient can also be increased via quantum confinement due to nanostructuring. Thus, nanostructuring with doping is an efficient way to enhance the 'figure of merit' of Bi₂Te₃ thermoelectric applications.

B1-0048

Magnetic, UV-visible and Dielectric Study of Cu_{0.8-x}Zn_xCr_{0.2}Fe₂O₄ System

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Abstract. Polycrystalline Copper-Zinc-Chromium ferrite with $Cu_{0.8-x}Zn_xCr_{0.2}Fe_2O_4$ System $(0.0 \le x \le 0.6)$ specimens were synthesized by solid state reaction method. The effect of Zn substitution on the structural, magnetization and UV-visible and dielectric studies was performed. The formation of single phase spinel structure was confirmed by X – ray diffraction (XRD) analysis. The lattice constant is increasing with zinc concentration and x-ray density decreasing simultaneously. Grain size of all specimens is found approximate 35 nm. The magnetic moment is found 1.774 to 0.165 bohr magnetron. The saturation magnetization Ms decreasing from 41.63 to 3.9 emu/gm. UV-visible measurements were recorded the maximum absorption was found at wavelength 231 nm to 219 nm and direct optical band gap found 3.58 eV to 3.74 eV. Dielectric properties was determined with the help of inductance-capacitance and resistance (LCR) meter.

Microhardness Studies of Poly (Vinyl Chloride) PVC and Poly (Vinylidene fluoride-co-Hexafluoropropylene) PVDF-HFP Blends

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Abstract. In the present study, microhardness measurements have been carried out on Poly(vinyl chloride) PVC, Poly (vinylidene fluoride-co-hexafluoropropylene) PVDF-HFP and their binary blends in various wt % i.e. PVC: PVDF-HFP:: 95:05;90:10;85:15 and 80:20. The effect of load on the microhardness of the blend specimens was studied by a Vicker Microhardness tester attached to a Carl Zeiss NU-2 Universal microscope. The curves obtained the effect of load on the microhardness level of the blend and variation on hardness with varying wt% of PVDF-HFP in pure PVC. The microhardness of the blends is found to decrease with increasing weight % of PVDF-HFP in blend samples. This is primarily due to plasticization effect which increases the chain flexibility and the elastic characteristics of the blend. Keywords: PVC, PVDF-HFP, Vicker Microhardness.

B1-0050

Sustainable Cubic CsPbI₃ Perovskite Active Layers in Open Air Environment

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Abstract:

Inorganic CsPbI₃ perovskite-based solar cells have attracted much attention from researchers because of their comparable photovoltaic performance and enhanced thermal stability compared to their organicinorganic hybrid perovskite counterparts. The desired cubic (α-) CsPbI₃ perovskite has a natural tendency to transform to the undesired orthorhombic (δ -) phase in ambient air conditions and so, it is required to prepare under a controlled air-free environment at a high temperature (320 °C). Therefore, the novelty of the work is that we have successfully prepared α-CsPbI₃ thin film in ambient air conditions at a comparatively low temperature (120 °C) through additive engineering. The preliminary X-ray diffraction pattern study indicates that cubic crystal system with $P\overline{m}3m$ space group obtained from the α phase of CsPbI₃ perovskite thin layers. The UV-Vis absorption spectroscopic study provides the absorption edge at ~ 693 nm corresponding to the sustainability of the cubic phase of CsPbI₃ perovskite. Furthermore, the steady-state photoluminescence (PL) spectroscopy displays the appearance of PL emission intensity at 700 nm. Thus, the energy bandgap of the α-CsPbI₃ perovskite (E_g=1.788 eV) obtained from UV-Vis spectroscopy exactly matches the bandgap obtained from PL spectroscopy. Therefore, the sustainable and cost-effective CsPbI₃ perovskite thin films obtained in an ambient environment and comparatively low-temperature conditions may be very effective active layers for perovskite solar cells.

Impact of Carbon Dots On Ionic Relaxation Of Nematic Liquid Crystal (6CHBT)

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Abstract. We report here the impact of Carbon dots (CDs, diameter ~7-8 nm) on the ionic relaxation of a homogeneously aligned nematic liquid crystal, namely, 4-(trans-4'-n-hexylcyclohexyl) isothiocyanatobenzoate (6CBHT) using the high-resolution dielectric spectroscopy. To investigate the effect of frequency, external DC bias, temperature and dopant (CDs) concentration on the ionic relaxation of 6CHBT, the tangent loss factor (tan δ) is greatly investigated. For instance, at room temperature, the frequency dependent tan δ clearly shows the significant shift in ionic relaxation of 6CHBT towards higher frequency with increase in the dopant concentration. The largest shift in the relaxation frequency is observed in case of 0.5 wt% CDs-6CHBT composite (i.e., highest concentration of CDs in the present study) and attributed to the change in molecular alignment of 6CHBT from planar to vertical due to dopant CDs. The temperature dependent studies show that frequency of ionic relaxation increases monotonically with temperature as expected and the magnitude of the shift is largest for 0.5 wt% CDs-6CHBT composite. To understand more about the significant shift in ionic relaxation frequency, the activation energy of ionic relaxation is calculated for all composites using Arrhenius plot and discussed its concentration dependence. We believe that our results would further shed more light on the present understanding of the dynamics of ionic relaxation in pure 6CHBT and its nanocomposites and useful for the development of advanced soft composite materials with tunable dielectric properties.

B1-0052

Evaluation of the photodegradation of organic pollutants in water using a highly visible lightactive tungsten oxide embellished graphitic carbon nitride

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Abstract. The coupling of semiconductor photocatalysts is a promising technique for reducing rapid recombination of photo-generated electron-hole and improving the separation of photoinduced charges in photodegradation processes. Rare earth metal oxide i.e., tungsten oxide is used to modify graphitic carbon nitride, also known as WO₃@g-C₃N₄ (WCN), were created in the current study by employing inexpensive urea and tungsten oxide powder as precursor materials. SEM (scanning electron microscopy), XRD (X-ray diffraction), FTIR (Fourier-transform infrared spectroscopy), as well as TGA (Thermogravimetric analysis) was utilized to describe the morphological characteristics, optical characteristics, and structural characteristics of the treated photocatalyst. Because of its potential use in photocatalytic environmental pollution remediation, graphitic carbon nitride (g-C₃N₄), a metal-free photocatalyst, has received a lot of interest. The results demonstrate that does not alter the crystalline structure of the sample but instead increases the surface area of g-C₃N₄ by dispersing it widely. Three different photocatalytic composites of tungsten oxide and g-C₃N₄ in the mass ratios of 1:1, 2:1, and 3:1, denoted WCN1, WCN2, and WCN3, were created for the methylene blue (MB) and methyl orange (MO) photodegradation. The combined photocatalytic degradation rate of MB after 150 minutes in visible light (500-800 nm) was 86.4% for WCN1, 98.8% for WCN2, and 91.2% for WCN3. For methyl orange, the photocatalytic activity of produced materials was also investigated. The analysis's outcome reveals astonishing deterioration values for WCN1 (72.9%), WCN2 (89.7%), and WCN3 (83.6%), respectively. The hybrid photocatalyst produced stable photodegradation performance for five cycles.

The heterojunction WO₃/g-C₃N₄ photocatalyst is a promising visible light active material for the treatment of pharmaceuticals and dyes in water using the photocatalysis process.

B1-0053

Green and Traditional Synthesis Of Copper Oxide And Its Effect On Optical Properties and Photocatalytic Dye Degradation Activity of CuO

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Abstract. Green synthesis of metal oxides has engrossed a significant attention because of its inexpensive procedures and environmentally friendly synthetic methods. In the present paper, we report the synthesis of Copper Oxide (CuO) by using orange peel and by conventional co-precipitation method and studied the properties of both the synthesized materials by XRD, FTIR, UV-Vis spectroscopy, SEM, and PL techniques. The results of XRD for both the samples confirm the pure monoclinic structure of CuO. FTIR shows the formation of Cu-O bond. The UV-Vis spectra show blue shift of the absorption peak. PL spectra of CuO shows emission near blue region. The Tauc plot is obtained to calculate the Band gap of both the samples. The photocatalytic activity of both samples has been monitored by Using UV spectroscopy. Green synthesized and conventionally synthesized CuO both exhibited high potential for the degradation of water-soluble industrial dye (Malachite Green).

B1-0054

Thermoelectric transport study in a small heterocyclic B₂C₂N₂H₆ molecule: A quantum many-body approach

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Abstract. Molecular electronics (ME) is a branch of science that investigates the electronic and thermal transport properties of circuits that use individual molecules as basic building blocks. This area of research has attracted a lot of interest due to its potential applications in nanoscale electronic devices like transistors, rectifiers, and switches. Here, we implement a combined quantum many-body approach and kinetic (master) equations to investigate transport properties in a weakly coupled molecule, B₂C₂N₂H₆. Several non-linear current-voltage characteristics, including negative differential conductance (NDC), rectifications, and the Coulomb staircase have been obtained in the specific coupling geometry of the molecule. We focus further on the thermoelectric property-based study as the development of high-performance thermoelectric materials and equipment recycles waste heat into electricity. Here, we investigate the thermoelectric transport through the B₂C₂N₂H₆ molecule with different coupling geometry in the linear response regime and explore possible conductance and thermopower coefficients with varying the Fermi energy of the electrode. The electrical conductance (G_V) peaks appear when the energy required for the transition from the N-electron state to the N+1electron state equals the Fermi energy of the electrode and the probabilities of occupying either electronic states are exactly equal. Again, electron waves traveling along the two branches of the B₂C₂N₂H₆ molecule may experience a relative phase shift. As a result, there may be constructive or destructive interference due to the superposition of the electronic wave function across the various pathways. So, there could be some antiresonance behavior as well as a change in electrical conductance. The thermal coefficients (G_T) give zero where the G_V has peaks because an electron transition occurs at specific Fermi energy, resulting in an electrical current but no net energy transport. Materials with low thermal conductance are used to create a compelling and reliable thermoelectric device. The advantage of molecular systems is that they may contribute very little phonon to thermal conductivity. The electronic contribution then largely determines the thermal performance. B₂C₂N₂H₆ molecule exhibits low electronic thermal conductance (ke) with high electrical conductance which has been beneficial for improving the thermoelectric performance. More interestingly, whenever a molecular orbital crosses the Fermi energy, the molecular occupation changes by one, and the sign of thermopower (S) changes. This is due to the switch from electron to hole-dominated transport whenever the Fermi

level has been crossed. The inverse relationship between conductance and thermopower exhibits fluctuating behavior in the figure of merit (ZT). we noticed that this small heterocyclic B₂C₂N₂H₆ molecular junction might be beneficial for upcoming thermoelectric devices.

B1-0055

The Electronic Transport Properties of CrSi₂/Si₉₈B₂ Composite: The Mid to Low Temperature Applications

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Abstract. In the mid-temperature region, Chromium disilicide is turning out to be a potential p-type thermoelectric material for utilizing the waste heat for power generation applications. Chromium disilicides are abundant in nature, less toxic, and have low-cost constituent elements. In the present work, $CrSi_2/Si_{98}B_2$ composite samples were synthesized using spark plasma sintering by dispersing ball-milled nanoparticles of $Si_{98}B_2$ with arc melted $CrSi_2$ powder. X-ray diffraction was used to identify the phases of the synthesized composites and to confirm this Rietveld refinement was performed. A field emission scanning electron microscope was used to examine the surface morphology of the samples. The inclusion of $Si_{98}B_2$ nanoparticles in the $CrSi_2$ matrix leads to a significant enhancement in the power factor $\sim 2.36 \times 10^{-3} \text{ W/mK}^2$ of the $CrSi_2/2\text{wt}\%$ $Si_{98}B_2$ composite at room temperature (323 K). However, the power factor peak of pristine $CrSi_2 \sim 1.4 \times 10^{-3} \text{ W/mK}^2$ was achieved at 423K. Here, the maximum power factor point shifted from mid temperature regime to low temperature regime which can be attributed to the optimization of the charge carrier concentration and mobility on dispersing 2 wt% $Si_{98}B_2$ into the $CrSi_2$ matrix. As a result, the $CrSi_2$ based thermoelectric materials can be used in low temperature applications.

B1-0056

Physical characterization of potassium modified lead bismuth borate glass system Divya^{a,*} Rajni Bala^a

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Abstract. A quaternary glass system for composition $xK_2O \cdot 20PbO \cdot (25-x)$ Bi₂O₃·55B₂O₃ with x=5, 10, 15, 20 and 25 was synthesized using melt quench technique and their physical properties were studied. To examine the effect of K_2O parameters like density (ρ), molar volume (V_m), crystalline volume (V_c), interionic distance (R_i), polaron radius (R_p), oxygen packing density (OPD) and field strength (F) were calculated. The calculated values of density and molar volume shows a decreasing pattern as the potassium oxide percentage increase. This decrement in density ascribed to replacement of Bi₂O₃ by K_2O content. Lower values of V_c from V_m show the existence of glass formation rather than crystallization.

Solid-state Symmetrical Supercapacitor Using Chemically Modified Multiwalled Carbon **Nanotubes**

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Abstract. Using multi-walled carbon nanotubes (MWCNTs) that were purchased commercially, new knowledge was discovered on the mechanism of porosity growth following chemical activation by KOH. Chemical activation was used to create activated multi-walled carbon nanotubes (A-MWCNTs). which have well-developed pore architectures and can be used as energy storage materials. The A-MWCNTs' microstructure and crystallinity were assessed using Raman spectroscopy and X-ray diffraction. A-MWCNTs' textural characteristics were examined using nitrogen gas sorption analysis at 77 K. The A-MWCNTs sample activated at 800 °C was found to have the maximum energy storage capacity. Its narrowest microporosity, which is strongly related to the energy storage capacity, was attributed to this. This demonstrates how pore volume affects energy storage behavior. Even though a large pore volume is desirable for storing energy. The precursor reacts with KOH, destroying the nanotubular shape. Only with KOH, which produced a significant number of flaws in the nanotube walls, are activation effects visible. It has been demonstrated that metallic K is easily intercalated. The well-conducting nanotubular material's open mesoporous network enables simple ion access to the electrode/electrolyte interface. The A-MWCNT-based solid-state supercapacitor device has an extended voltage window with high specific capacitance and exhibits excellent cyclic stability even after 10,000 cycles. In this instance, the specific capacitance of the nanotubular electrode material is increased up to 193 F/g in the potential range of 0-1 V from GCD data at a current density of 0.5 Ag⁻¹, and microporosity was significantly improved.

B1-0058

Effect of NaPF₆ on the ion transport properties of Sodium alginate (NaAlg)-Poly (vinyl alcohol) (PVA) solid bio-polymer blend electrolytes

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Abstract. This research focuses on systematically exploring the impact of NaPF₆ doping on the structural, electrical, and thermal attributes of a biodegradable blend comprised of sodium alginate (NaAlg) and poly (vinyl alcohol) (PVA). XRD analysis highlights an overall reduction in the blend's crystallinity. FTIR spectroscopy unveils salt complexation with the polymer matrix's polar groups through coordinate bonds. Room temperature Electrochemical Impedance Spectroscopy (EIS) discloses a remarkable three-order increase in ionic conductivity (10⁻⁵ S/cm) compared to the pure blend. Employing Nyquist plot fitting and an electrical equivalent circuit, transport parameter variations are studied, emphasizing the significant role of carrier concentration in conductivity. Transference number measurements, utilizing the Wagner polarization technique, indicate that ions are the primary charge carriers. This suggests the potential use of the optimized sample as a separator or electrolyte in energy storage devices, particularly with further enhancements of ionic conductivity.

Enhanced Visible-Light Driven Photocatalytic Activity of ZrO₂/g-C₃N₄ Nanocomposites towards Organic Pollutants

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Abstract. In the present work a three-step process has been performed to synthesize Zirconium Dioxide doped Graphitic Carbon Nitride (g-C₃N₄-ZrO₂) nanocomposite photocatalyst. In the first step g-C₃N₄ was synthesized by simple calcination process using Urea. In the second process Zirconium dioxide (ZrO₂) was synthesized by simply calcining Zirconium Oxychloride Octahydrate (ZrOCl₂.8H₂O). In the third step, we synthesized Graphitic Carbon Nitride (g-C₃N₄) based ZrO₂ doped nanocomposite materials with varying mass ratios (g-C₃N₄:ZrO₂- 1:1, 2:1, 3:1). SEM (scanning electron microscopy), XRD (X-ray diffraction), FTIR (Fourier-transform infrared spectroscopy), as well as UV-Vis spectroscopy was utilized to describe the morphological characteristics, optical characteristics, and structural characteristics of the treated photocatalyst. FTIR spectra revealed the presence the functional group thereby confirming the formation of composites. FE-SEM analysis performed to study the morphological aspects of the synthesized nanocomposite photocatalysts. The combined photocatalytic degradation rate of MB after 150 minutes in visible light (500–800 nm) was 76.4% for g-C₃N₄-ZrO₂ with 2:1. The synthesized photocatalyst holds a bright scope for the efficient remediation of organic.

B1-0060

Combustion Synthesis, Rietveld Refinement and Optical Studies of Calcium Titanate (CaTiO₃) Perovskites

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Abstract. Calcium Titanate (CaTiO3) perovskites were synthesized by the modified combustion method. This synthesis method is self-sustained due to its exothermic and auto-catalytic features which means once initiated it will ultimately convert precursor into product with high purity, minimized segregation, and sound monitoring of the resulting perovskite composition. The structural information of the prepared sample was obtained by X-ray diffraction Rietveld refinement and the W-H plot was used to determine the microstrain and the average size of the particle. The output file generated after refinement was used to develop the crystal structure. Diffuse reflectance UV- Visible spectral studies gave the optical band gap as 3.65 eV, which implies that the sample falls under the category of wide band gap semiconductors

Effect of Sonication Time on Synthesis of MoS₂ Nanosheets

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Abstract. MoS₂ is a kind of transition metal dichalcogenide (TMD) that has a single atom of molybdenum bonded to a pair of sulfur atoms. Through its unique and diverse superior properties, it has challenged the supremacy of graphene and related 2D materials and thus has emerged as a front runner in the development of miniaturization and wearable electronics for various applications. In the present work, MoS₂ nanosheets have been synthesized from the bulk MoS₂ powder through exfoliation using bath ultrasonication for two different times in ethanol and deionized (DI) water. It results into formation of mono/multilayer MoS₂ nanosheets. The results are confirmed by UV-VIS spectroscopy. It is seen that the absorption intensity decreases with increase in sonication time from 1 hour to 2 hours. However, the position of the two signature peaks is almost unchanged. The results are discussed to explain average layer numbers as well as size/thickness of MoS₂ nanosheets.

B1-0062

Electrodeposited CoP nanoparticles for bifunctional water electrolysis

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Abstract. An efficient method of addressing the energy crisis and environmental issues is the development of high-efficiency catalysts for bifunctional water electrolysis with simultaneous generation of hydrogen (H₂) and Oxygen (O₂) gas. The transition metals with significant reserves and their phosphides are becoming intriguing Pt, RuO₂ substitutes for the water splitting process. Herein, we report the fabrication of a self-supported mesoporous array of CoP nanoparticles on nickel foam (CoP/NF) via a one-step electro-deposition technique and their characterization for overall water splitting in both acidic (0.5M H₂SO₄) and alkaline (1M KOH) solutions. The as-prepared electrode required only 235 mV and 330 mV overpotential to achieve 500 mA/cm² current density for HER and OER respectively in an alkaline solution. Encouragingly, CoP/NF generates an extremely high current density of 1700 mA/cm² at 200 mV. The efficient electronic transport as well as the porous structure of foam that provides a large electrochemical active surface area (ECSA) are responsible for the exceptional performance of the CoP/NF. Furthermore, a two-electrode water electrolysis cell produces 1000 mA/cm² at a voltage of 1.86 V at 25°C and just 1.71 V at 80°C. These findings support the creation of reliable and effective electrodes for the production of green hydrogen (H₂) on an industrial scale.

Application of PZT in Civil engineering

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Abstract. Civil engineering is not just about construction of buildings, towers, bridges etc. but also of their caring and maintenances. For this purpose all the constructed structures have to be monitored for their structural health in terms of damage detection, severity of damage etc., collectively called structural health monitoring (SHM) of structures in civil engineering. For SHM, electromagnetic impedance (EMI) technique is one of the best methods of NDTs [25] being used in the field of civil engineering. EMI uses lead zirconate titnate (PZT) as its piezoelectric component for the purpose of measurement. PZT based devices are widely used in civil engineering. There is a huge demand for health monitoring now a days and to full fill those demands of health monitoring, PZT is one among the most reliable and cost efficient material. Piezoelectric sensor can be used to measure changes in acceleration, strain, pressure and to ensure the better safety measures. These PZT based sensors can be used for predicting the natural disasters like earthquake that helps to save the thousands of lives and can decrease property lose. The piezoelectric sensors can be used to monitor the civil structure which helps an engineer to analyses the characteristics of that structure. It is also used for collecting the data of force that is being exerted on the ground by the building, temperatures and pressure differences in environment etc. Damage detection is a technique that is used to monitor the civil structure, this can improve safety and ensure durability, and for concrete structures, damage detection plays an important role.

For the purpose of SHM and damage detection PZT based sensors can be used. For civil engineering applications PZT-cement based composites has been developed. The concrete and host structure such PZT-cement based composites shows better matching when compared to normal or other piezoelectric ceramics. In this review work we have discussed about SHM/Damage detection, Vibrational control, PZT embedded cement composites and PZT embedded in concrete.

B1-0064

Self-supported Cr doped NiFe2O4 electrocatalysts for Overall water splitting

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Abstract. The development of efficient nanostructured electrocatalysts utilizing non-noble metals holds enormous prominence for water electrolysis. We report the fabrication of a Cr doped NiFe2O4 Nanoparticles on 3D nickel foam using a two-step synthesis route (hydrothermal and annealing). Herein, Cr-NiFe2O4@NF electrocatalysts has been explored for overall water splitting. Electrodes require the over potential of 165 mV for HER and 230 mV for OER to achieve the current density of 10 mA/cm2 in 1M KOH. Different electronic states of metallic elements additionally create a synergistic phenomenon that advances the rate of electrochemical reactions during water electrolysis. The electrochemical surface area (ECSA) is significantly enhanced on Cr-doping, which further enhances the rate of hydrogen and oxygen generation. Furthermore, the Cr-NiFe2O4@NF electrodes shows stable HER and OER performance for more than 24 hours.

A Review on magneto-electric characterises of Co-modified PZT

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Abstract. This review article explores the magneto-electric characteristics of Co-modified PZT (Lead Zirconate Titanate) materials. Co-modified PZT materials have gained considerable attention in recent years due to their unique ability to couple magnetic and electric properties. The addition of cobalt ions introduces magnetic moments into the material, leading to enhanced magneto-electric coupling. This review discusses the tailoring of magnetic and electrical properties in Co-modified PZT, the emergence of multiferroic behaviour, and the applications of these materials in sensing, actuation, and energy harvesting. The review also highlights the challenges in optimizing the material's composition, stability, and scalability for practical applications. Overall, Co-modified PZT materials offer promising opportunities for the development of advanced multifunctional devices and hold great potential for future research and advancements in the field.

B1-0066

Self-supported Cr-Cu₂S Nanoflakes for Hydrogen Production from Seawater with industrial scale Current Density

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Abstract. Herein, we report the one-step hydrothermal synthesis of bifunctional Cr-Cu2S Nanoflakes supported on Cu-foam (Cr-Cu2S@CF) for alkaline water electrolyzer for H2 production at an industrial scale. Vertically oriented Cr-Cu2S Nanoflakes, forming a hierarchical network is capable of efficient electrocatalytic activity owing to the high surface area, effective ions channels, and abundant redox sites. Owing to advanced morphological features, Cr-Cu2S@CF demonstrates the binder-free electrocatalytic hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) at an industrial scale high current density of 500 mA/cm2. Exploiting the synergistic features, the optimized chemical composition of Cr-Cu2S delivers the geometric current density of 100 mA/cm2 at overpotential of -407 and -350 mV for HER and OER activity, respectively. Alloying Cr in Cu2S networks enhances oxygen desorption at the anode by decreasing the energy of adsorption of *OH intermediates, apart from enhanced HER activity due to enhanced electron density at Cu-sites. Moreover, two a two-electrode electrolyzer assembled using Cr-Cu2S@CF as an electrocatalyst at both electrodes gives current densities of 10 and 100 mA/cm2 at potentials of 1.75 and 2.07 V, respectively.

PZT as an Electronic Material

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Abstract. Piezoelectric materials play a crucial role in numerous electronic applications, offering unique properties that enable the conversion of mechanical energy into electrical signals and vice versa. For *m*ore than a decade, lead zirconate titnate (PZT) has been among the most extensively utilized and researched piezoelectric ceramic that shows versatile characteristics with different composition and dopants. PZT is one of the materials which can show high dielectric constant, remnant polarization and can operate at low voltages. In this review article, we explored various electronic applications of PZT. In this work, some synthesis methods and composition, suitable for electronic applications of PZT has been presented in this review article. Alongwith a comprehensive study of PZT as an electronic material for energy harvesting, MEMS, RAMs and VLSI applications.

B1-0068

A study on Magnetio-Electric Characterization of Fe-Doped PZT

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Abstract. This review paper provides a comprehensive analysis of the magnetoelectric (ME) characterization of iron-doped lead zirconate titanate (Fe-doped PZT). The ME effect, involving the interplay between magnetic and electric properties, is investigated. The review covers synthesis methods, characterization techniques, and factors influencing the magnetoelectric response. In the synthesis section, the paper discusses the different approaches used to incorporate iron into the PZT lattice, emphasizing the role of doping concentration and processing parameters in optimizing the magnetoelectric behavior. Characterization techniques such as electrical, magnetic, and magnetoelectric measurements are extensively covered, providing insights into the mechanisms governing the observed coupling phenomenon. Furthermore, the review explores the factors influencing the magnetoelectric response in Fe-doped PZT, including compositional variations, domain structure, defect engineering, and interface effects. The paper investigates the influence of external factors such as temperature, electric field, and magnetic field on the magnetoelectric properties, shedding light on their impact. The review concludes by discussing potential applications of Fe-doped PZT in various fields, such as spintronics, sensors, and energy harvesting. It also highlights the need for further research to optimize the magnetoelectric performance and explore novel fabrication techniques.

Small angle neutron scattering studies of PVB-MWCNT Nano composites

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Abstract. Due to the significant role played by polyvinyl butyral (PVB) in laminated materials, it is crucial to conduct comprehensive investigations into the surface and structural characteristics of PVB and its composite materials. The Kratky plot exhibited positive deviation. Each sample exhibited a positive deviation, suggesting that the polymer chains experienced swelling, regardless of whether the sample consisted solely of PVB or a mixture of PVB and MWCNT. Furthermore, it was observed that the PVB+1.0wt%MWCNT sample exhibited a greater positive deviation, indicating that the extent of swelling would escalate with an increase in the MWCNT concentration in PVB. The estimation of the surface fractal dimension of nanoparticles was conducted by using data acquired from Small-Angle Neutron Scattering (SANS) technique. The results of the study suggest that the PVB+MWCNT composite displays elevated levels of roughness and swelling in comparison to the pure PVB material.

B1-0070

Design and Development Of Supercapacitor For Hybrid Energy Storage System

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Abstract. Design and fabrication of novel carbon-based materials for flexible energy storage devices has become very feasible as the electrochemical performances of studied concerned electrode materials such as TMOs, nanostructured carbon-materials, electrically conducting polymers, nanocomposites, and various electrolytes such as organic, aqueous, ionic liquid, solid electrolytes, etc., are compared and discussed in various publications. Number of different materials are observed and studied which can contribute for fabrication of enhanced Super-capacitor. Here are some of the synthesis methods such as Chemical Oxidation process, thermal pyrolysis, hydrothermal method, etc., along with diverse characterization techniques which includes XRD, FESEM, TEM, FT-IR, EDX etc. Major findings of current research's Future perspectives which includes enabling working on the clean energy materials Innovation confronting to push the innovation process of new excellent performance, economical clean energy materials. Various types of electrodes and electrolytes are utilized to study different electrochemical properties and its enhancement for Super-capacitor fabrication. It Can be used in various application such as renewable energy integration, Energy harvesting, smoothens output power by renewable energy storage, balances generation-demand load with facile load profile, improving the power quality.

Enhanced Electrochemical Performance of Cr-Doped YCr_xMn_{1-x}O₃ Perovskite Oxides as Electrode Materials for Supercapacitors

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Abstract. The field of supercapacitors has attracted significant attention as a promising solution for energy storage in recent years. Among various electrode materials, perovskite oxides (ABO₃) become the material of choice, this choice is due to their stable crystal structure and their inherent oxygen vacancies which tune their electronic properties, leading to improved electrochemical performance. In this study, we synthesized pristine and Cr-doped YCr_xMn_{1-x}O₃ perovskite oxides and conducted a comprehensive investigation of their electrochemical properties. Electrical measurements of the electrodes demonstrated increased conductivity after Cr doping. The YCr_xMn_{1-x}O₃ (x=0.1) material exhibited the highest specific capacity of 492 mAh g⁻¹, attributed to enhanced electrolyte diffusion and ion intercalation during surface redox reactions, facilitated by the improved electrode conductivity and the presence of oxygen vacancies.

B1-0072

Effect of Trivalent Rare Earth substitution (Ho, Eu) on Structural Properties of Bismuth Ferrite Multiferroic

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Abstract. Polycrystalline materials with composition Bi_{0.9}A_{0.1}FeO₃ (A = Ho, Eu) were synthesized by conventional solid state reaction method. Structural investigation of the sintered ceramics is done by powder X-ray diffraction at room temperature. Reitveld refinement done by FullProf program presented good agreement between observed and calculated pattern. Refinement also revealed no change in crystal structure on 10% substitution of trivalent ion (Ho, Eu) at Bi site. All the samples crystallized in rhombohedral structure with space group R3c as of parent BiFeO₃. Substitution at Bi site reduced the formation of secondary phases (Bi₂Fe₄O₉ and Bi₂₅FeO₄₀) and no traces of Ho₂O₃ and Eu₂O₃ have been found up to 10 % substitution. The crystal structure will change from high symmetric state to low symmetric state as average ionic radii at Bi site decreases as evident from Goldschmidt tolerance factor.

Structural and electrical properties of ZnO doped NKBN piezoelectric ceramic prepared by solid-state reaction technique for electronic application.

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Abstract. Ceramic materials based on the composition 0.98(Na_{0.5}K_{0.5}NbO₃) + 0.02(Sr Bi_{0.5}Nb_{0.5}O₃) + x ZnO (x=0, 0.20, 0.30, 0.45, 0.60) have been synthesized through a solid-state reaction method and characterized to explore their unique properties and potential applications. In this study, we investigated the influence of varying "x wt% ZnO values on the physical, electrical, and structural characteristics of Na-K-Nb-O and Sr-Bi-Nb-O matrix (coded as NKBN) ceramics. Our results reveal that the addition of ZnO to the NKBN ceramics has a significant impact on the dielectric and impedance properties of the ceramics. Depending on the "x value of ZnO," we observed variations in dielectric constant, dielectric loss, and ferroelectric hysteresis loops. Furthermore, the structural analysis using techniques such as X-ray diffraction and scanning electron microscopy showed that the crystal structure and microstructure of the ceramics were strongly influenced by the ZnO content, affecting their mechanical and thermal properties. The electrical conductivity of the ceramics also exhibited a dependence on ZnO content, making them suitable for a range of electronic devices. The tunability of their properties through the manipulation of "x wt% of ZnO concentration" makes them versatile candidates for next-generation electronic and electromechanical devices.

B1-0074

Harvesting the NIO nanoparticles decorated Polyaniline thin film and Investigation the diverse properties

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Abstract. Present study reported the effects of NiO nanoparticles on the structural, optical and morphological properties of polyaniline (PANI) thin film. Pure PANI and PANI-NiO thin films were prepared by soft chemical route in HCL aqueous solution. The structural, optical and morphological properties of the developed thin films were characterized via X-ray diffraction (XRD), ultraviolet-visible (UV-vis.) spectroscopic and Field emission scanning microscopy (FE-SEM) techniques respectively. XRD study shows the amorphous nature of both pure PANI and PANI-NiO thin films. NiO nanoparticles not merely effects the structural properties of the PANI due to the small doping quantity. UV-vis. absorption spectrum of PANI shows the two absorption peaks at approximately 370 nm and 472 nm, respectively. In PANI-NiO nanocomposite, the absorption peaks slightly shifted due to the interaction of the NiO with the PANI molecules. PANI shows agglomerated form and due to the doping of NiO, PANI-NiO shows the aggregated globular surface morphology.

Effect of cold working and annealing on micro hardness of $InBi_{1-x}Te_x$ (x=0, 0.05, 0.1, 0.15) Crystals

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Abstract. Indium bismuthide is a well-explored group III-V semi-metallic compound for IR technology applications. Here we report mechanical properties of this low band gap crystals using Zone melting method. The crystals of $InBi_{1-x}Te_x$ (x=0.05, 0.1, 0.15) were grown using Zone-melting method with 0.3cm/hr growth speed and 10 alternate zone passes. In the present work the microhardness of these crystals with the above said composition range has been investigated. The hardness has been studied with respect to applied load as well as of the composition of the crystal, at room temperature. $InBi_{1-x}Te_x$ (x=0.05, 0.1, 0.15) crystals exhibit impurity hardening as compared to the pure InBi crystal. Hardness tests were also performed on as-cleaved, cold-worked and annealed crystals. The impact of crystal perfection on microhardness has been studied and the detail results are reported. With increasing Te content, the hardness shows increasing trend.

B1-0076

Sol-Gel synthesis and crystalline size, dislocation density and microstrain of LiNi_{0.85}Co_{0.10}Mn_{0.05}O₂ cathode material for lithium-ion batteries

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Abstract: Lithium-ion batteries (LIBs) are essential energy storage solutions for a wide range of applications. The cathode material significantly influences the performance of LIBs. Nickel-cobalt-manganese (NCM) ternary cathode materials have gained prominence due to their potential to offer high capacity, stability and voltage characteristics. In this paper, we focus on the synthesis of NCM cathode material using sol-gel method and its characterization primarily through X-ray diffraction (XRD) analysis. The crystal structure of the synthesized material is investigated using XRD. These XRD patterns are analyzed to estimate particle size and to deduce crystalline size, dislocation density and microstrain. This study helps us better understand how NCM materials are put together, which is important for making high performance lithium-ion batteries. These batteries are used in laptops, electric cars, etc.

Study of Strain On Structural Stability and Electronic Properties of PdTiSn Half Heusler Compounds

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Abstract. Using density functional theory (DFT) structural, electronics characteristics and stability of half-Heusler PdTiSn compounds have been reported at various values of tensile strain. The calculated value of formation energy and phonon dispersion curve, confirm the chemical and thermodynamic stability of PdTiSn material at various amounts of isotropic strain. Calculations show that when different values of tensile strain are applied, the energy bandgap varies dramatically. The estimated outcomes reveal that these materials may be used in thermoelectric applications.

B1-0078

Comparative Analysis of Physical Properties of ANdFeTiO₆ (A = Sr, Ba) Double Perovskites

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Abstract. This study focusses on the synthesis of double perovskite oxides ANdFeTiO₆ (A = Sr, Ba) utilizing solid–state reaction method. X–Ray diffraction analysis revealed orthorhombic symmetry in SrNdFeTiO₆ and cubic symmetry in BaNdFeTiO₆ compounds. Dielectric investigations unveiled dispersion pattern and relaxation phenomena in both the samples, with BaNdFeTiO₆ demonstrating superior characteristics. Impedance spectra exhibited a negative temperature coefficient of resistance (NTCR) behavior in both the samples. Magnetic analysis demonstrated canted ferromagnetic behavior in SrNdFeTiO₆ and BaNdFeTiO₆ compounds. Substituting Sr atoms with Ba atoms resulted in an enhancement of magnetic moment in SrNdFeTiO₆.

At room temperature enhancing humidity sensing performance

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Abstract. In the present work, synthesised the turnery components to improve the sensing ability. By adding the Y_2O_3 to Fe-ppy composite, the humidity sensing capability is improved. The sample was prepared by using simple technique; mechanical vibration. The synthesised samples were analyzed by FTIR and XRD techniques. The stirrer liquid sample was deposited on the ordinary glass substrate by using simple cost effective method i.e spin coating method. The sensing performance of the turner film is good. It senses the humidity very quickly and shows the response and recovery times are 11s and 12s respectively at room temperature. The film works basically the formation of chemisorption and physisorption layers followed by capillary condensation process.

B1-0080

Synthesis and Thermoelectric Characterization of Higher Manganese Silicide based Thermoelectric material

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Abstract. Abstract. In the area of sustainable and green energy sources, thermoelectric power generation emerges as a scientifically promising and ecologically friendly technology. Thermoelectric technology effectively converts heat into electricity, harnessing various heat sources, including waste heat from industrial processes, sunlight, and even the human body. Despite its potential as a net-zero emission power generation technology, thermoelectric power generation needs to address some critical challenges, such as the use of non-toxic materials, improving material efficiency, and reducing production costs. Considering these challenges, Higher manganese silicide (MnSiy) is one of the most promising alternative materials containing cheap and non-toxic elements. The power generation efficiency of higher manganese silicide is ambitious for energy applications. To improve the figure of merit, we attempted stable Cu doping in higher manganese silicide employing state-of-the-art synthesis processes and techniques and synthesized Cu-doped and Cu and Ge double-doped HMS samples. Their crystallographic structures are subjected to meticulous examination, the intricacies of their morphological features are delved into, and their thermoelectric transport properties are subjected to rigorous analysis. The electrical transport properties of the synthesized materials were studied in the temperature range of 323 K to 873 K. The synthesized specimens exhibit a p-type degenerate semiconducting nature throughout the measurement. Cu doping improves the electrical conductivity; however, lowering the Seebeck coefficient results in a small improvement in the power factor. The (Cu, Ge) double-doping is more effective in improving the power factor because of its high electrical conductivity and Seebeck coefficient. The double-doping of Cu and Ge in HMS improves the power factor effectively to ~1.98 × 10-3 W/mK2. The (Cu, Ge) double-doping in HMS showed a higher calculated weighted mobility than the Cu-doped HMS. The high-power factor obtained through Cu and Ge double doping in HMS is highly beneficial for realizing its device application.

Effect of Temperature Change on Thermo-acoustic Parameters of Binary liquid mixture of Benzyl propionate with Ethanol

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Abstract. In this research article, density (ρ), speed of sound (u) and viscosity (η) of binary liquid mixtures containing benzyl propionate with ethanol were measured over the entire range of composition at temperatures 308 K, 313 K, 318 K, 323 K, 328 K and 333 K. The acoustic impedance (Z), adiabatic compressibility (β_a), Intermolecular free length (L_f), relaxation time (τ), internal pressure (π), and thermodynamic parameters like Gibb's free energy (ΔG) and enthalpy (H) have been calculated using experimental data. A discussion was carried out in terms of interactions and structure factors in this binary mixtures based on results obtained. The linear variations are found for the thermo-acoustic parameters which imply the presence of solute-solvent interactions in the binary system that strengthens the above findings.

B1-0083

Impedance Spectroscopic Studies on Six-layered Bi₇Ti₄NbO₂₁ Aurivillius Intergrowth Ferroelectric Ceramic

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Abstract. Intergrowth materials are found to use in the advanced ferroelectric memory and pyro sensing devices. The present Aurivillius phase compounds are generally expressed with the molecular formula as: $(Bi_2O_2)^{2+}$ $(A_{n-1}B_nO_{3n+1})^{2-}$. Here the term 'n' represents the number of $(A_{n-1}B_nO_{3n+1})$ perovskite units. The perovskite blocks of structure of the compounds were interleaved between perovskite blocks and bismuth oxide $(Bi_2O_2)^{2+}$ layers. The said above slide slipping intergrowth compounds are generally prepared by addition of n-layered and (n+1) layered compounds. Moreover the plausible reason for getting enhanced ferroelectric properties in the intergrowth structure seems to be an attractive study. Moreover the relationships between the intergrowth structure and their constituent layer compounds have been rarely studied. Based on our earlier results and other reports suggested that intergrowth compounds have positive effects on their ferroelectric properties. Keeping this in view, an attempt is made in the present study focused on electrical properties.

In the present investigation a six layered compound, namely $Bi_7Ti_4NbO_{21}$ was prepared by adding the three-layered compound ($Bi_4Ti_3O_{12}$) and two layered compound (Bi_3TiNbO_9) by means of intergrowth route. The product compound belong to orthorhombic structure and the lattice parameters (a =5.442 A^0 , b =5.404 A^0 , c = 57.990 A^0) were evaluated. Dielectric and impedance studies we are measured with the help of HP 4192A analyzer. A detailed study on conductivity, impedance, dielectric and complex impedance analysis was carried out on the said above intergrowth compound, and the results are discussed.

Structural and Photoluminescent Properties of Dy³⁺ doped Ca₂Ga₂SiO₇ Phosphor for White Light Emitting Diodes

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Abstract. Dy³⁺ doped Ca₂Ga₂SiO₇ were prepared via conventional solid-state reaction technique and characterized for structural and photoluminescent properties. The XRD analysis confirm the presence of single-phase tetrahedral structure of Ca₂Ga₂SiO₇ belonging to P4⁻21 m space group. Under the n-UV excitation, mainly two stronger emission peaks in the blue band and the yellow band, which correspond to the electron transitions at ${}^4F_{9/2} \rightarrow {}^6H_{15/2}$ and ${}^4F_{9/2} \rightarrow {}^6H_{13/2}$ of Dy³⁺, respectively were observed. The final phosphor emission falls in the white light region, as indicated by the CIE chromaticity coordinates and the CCT values. The optimal doping concentration of Dy³⁺ in Ca₂Ga₂SiO₇ host matrix was obtained and the main mechanism of concentration quenching in the sample was dipole–dipole energy transfer, as evident from the results of Dexter theory. The above-mentioned results clearly indicated that Dy³⁺ doped Ca₂Ga₂SiO₇ has potential application in the white light emitting diodes.

B1-0085

DBD treated PVA/Aloe Vera Nanofiber As A Novel Dressing Platform

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Abstract. Atmospheric dielectric barrier discharge (DBD) has gained recognition as a practical technique for modifying the surface properties of polymers. With its ability to alter the chemical and physical properties of material surfaces at room temperature without any change to their bulk properties, there has been notable interest in the advancement of innovative wound dressings. Aloevera, recognized for its ability to naturally break down, compatibility with the body, and minimal harmfulness, contains numerous bioactive substances that offer advantageous qualities such as antimicrobial, anti-inf lammatory, and immune-modulating effects. These qualities can effectively enhance the process of wound healing. For this study, 12 wt.% Polyvinyl Alcohol (PVA) is blended with Aloe vera gel at a ratio of 5:1. These fabricated nanofiber mats are subjected to DBD plasma treatment in oxygen (O2) gas at atmospheric pressure. The morphology of the produced nanofibers is examined using a Field Emission Scanning Electron Microscope (FE-SEM), which confirms the production of beads-free electrospun nanofibers. Additionally, various physical properties such as crystallinity, functionality, and mechanical strength of the nanofiber mat is assessed using techniques including Powder X-Ray Diffraction (PXRD), Attenuated Total Reflectance Fourier Transf orm Inf rared (ATR -FTIR) spectroscopy, and mechanical property testing. Furthermore, the contact angle of the nanofiber mat is measured before and after plasma treatment, and the results demonstrated satisfactory outcomes. The DBD plasma treated nanofibers shows relatively better antibacterial activities against Gram-negative Escherichia coli and Gram-positive Staphylococcus aureus bacteria. These findings suggest that the electrospun PVA/Aloevera nanof ibers treated with DBD plasma hold promise for utilization as wound dressings in the treatment of skin and wound infections.

Theoretical Estimation of L X-Ray Fluorescence Cross-Sections for ⁵¹Sb and ⁵²Te at 6 kev and 8 kev Excitation

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Abstract. Evaluation for L_{α} , L_{β} , L_{γ} , X-ray photo cross-section have been done for ⁵¹Sb and ⁵²Te at excitation energy 6 kev and 8kev. The theoretical values of the cross-sections were calculated using tabulated data sets of different physical parameters, such as L subshell photoionization cross-sections (PCS) σ_{Li} (i= α , β , γ), fluorescence yields (ω_{i}), coster-kronig transition probabilities (f_{ij}) and radiative decay rates (F_{ij}). DHS model with data set of Campbell and Puri was used to calculate L XRF cross sections. Theoretical data of these elements at this excitation energy are highly desirable in order to check the reliability of experimental results.

B1-0087

Preparation and Functional characterization of $Sr_XY_{1-x}Ti_XFe_{1-x}O_3$ composites (x = 0.0, 0.5 and 1.0)

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Abstract. The aim of this work was to prepare $Sr_XY_{1-x}Ti_XFe_{1-x}O_3$ composites (with $x=0.0,\ 0.5$ and 1.0) by modified solid state reaction method and to investigate the structure and hyperfine interactions of the material. Pure phase materials are synthesized using the solid state reaction method by combining the oxides of the constituent compounds. X-ray diffraction was applied as complementary methods. X-ray diffraction revealed that for both mixing techniques led to a partial eliminating of the impurities. Here, we used two methods to estimate coherent crystal size using the Debye Scherer and W-H diagram. In addition, the W-H diagram also provides the microtension present in the composite. Research on optical materials shows that the material is a wide-bandgap semiconductor that can be used to improve its dielectric properties.

Study of Stacking Fault Energy of Ni-Based Superalloy Using Density Functional Theory Calculations

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Abstract. Ni-based alloys or super-alloys are of great interest in potential applications such as aerospace and nuclear reactors. Particularly, Inconel 718 (IN718) has drawn much attention for the structural component in nuclear reactors due to its excellent properties, such as high temperature strength, ductility, good corrosion resistance and toughness [1]. During the operation of a reactor, the materials undergo radiation damage due to the energetic neutrons, resulting in loss of structural integrity and degradation of mechanical properties. Some of the important irradiation-induced microstructural changes are formation of defects clusters, dislocation loops, stacking fault etc. These, in turn, play a significant role on the mechanical strength of the material. Thus, to understand the effect of irradiation on the formation of these defects, Ab Initio calculation of defect formation energies in IN718 alloy was carried out. We have attempted to calculate particular the stacking fault energy (SFE) of individual alloying elements of IN718 in pure Ni and the IN718 itself. IN718 has a face-centered cubic (FCC) structure consisting of a regular stacking sequence ABCABC... along the closed packed {111} plane [2]. In the present study, all the calculations are performed using Vienna Ab-initio Simulation Package (VASP) based on the Ab Initio density functional theory (DFT) [3]. Here, Pardew-Burke-Ernzerhof (PBE) exchange-correlation functional has been used within GGA approximation with optimized plane wave cut-off energy of 450 eV and 3x5x1 k-point mesh. It is observed from the results that the stacking fault energy reduces by adding individual elements in Ni. The influence of the alloying elements on SFE is stronger in the combined effect of the alloying elements in IN718 than the individuals.

B1-0089

A review and tabulation for XRP cross sections for Oxygen and Carbon ion impact Vasu Khurana^{1*}, Shehla¹

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Abstract. The X-ray production (XRP) cross sections for Oxygen and Carbon ion impact have been extensively studied and measured for various target materials and ion energies. The results have important applications in a range of fields, including radiation therapy, space exploration, nuclear engineering, atmospheric and environmental science, and plasma physics. Experimental techniques for measuring XRP cross sections and theoretical models used to calculate cross sections have been discussed in this review. A tabulation of the XRP cross sections for different target materials and ion energies, along with information about the measurement or calculation method used for each data point, has been provided. The advantages and limitations of each measurement and calculation method have also been discussed. The presented data can serve as a valuable resource for researchers and engineers in various fields who require accurate and reliable XRP cross sections for Oxygen and Carbon ion impact. Overall, the review highlights the importance of understanding XRP cross sections for the development and optimization of a range of technological applications.

Investigation on Structural and Magnetic Properties of Cu Substituted Ni₂-X Hexaferrite

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Abstract. Using the method of heat treatment, a series of copper substituted X-type $Sr_{2-x}Ni_2Cu_xFe_{28}O_{46}$ (x = 0.0, 0.2, 0.4, 0.6, 0.8, 1.0) hexaferrites were prepared. XRD analysis shows the coexistence of X-type and W-type phases. Fourier-transform infrared spectroscopy (FTIR) analysis unveiled two distinctive absorption bands spanning the range of 410 cm^{-1} to 510 cm^{-1} . These bands are attributed to the stretching vibrations of Fe^{3+} - O^2 -, serving as conclusive evidence for the formation of the ferrite phase. A discernible trend was observed in the saturation magnetization (M_S) and coercivity (Hc) properties across the varying copper substitution with the highest values recorded at $58.580 \text{ Am}^2/\text{Kg}$ (x = 0.2) for M_S and 244.94 Oe (x = 0.0) for Hc. The hexagonal platelet morphology has been observed for all the samples through FESEM images. Moreover, the reduced remanence observed in the substituted compositions enhances their suitability for potential applications in transformer core production. This research opens up exciting avenues for the utilization of copper-substituted X-type hexaferrites in various technological domains.

B1-0091

On the Electrical properties and Temperature-dependent properties, viz., Viscosity and Relative density of Water-based Spinel Zinc Ferrite Ferro fluids

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Abstract. While studying thermo-acoustic properties of binary, ternary liquid mixtures or that of ferrofluids, one not only need to measure the variation of acoustic parameters like acoustic impedance, hydration number, Rao's constant, Wada's constant, apparent molar volume, apparent molar isentropic compressibility at different temperature values but also need to see whether parameters like relative density, viscosity of the substance changes with change in temperature. This study is of utmost importance because while estimating the acoustic parameters sometimes relative density, sometimes viscosity and sometimes both of it appears in the formula. Electrical properties of the substances are also of similar importance. Hence, investigation of variation of viscosity, relative density of specific ferrofluids, with temperature is an important area of study. In this communication we have reported variation of viscosity, relative density of water based Zinc Spinel ferrite with temperature. The electrical properties of the water based Zinc Spinel ferrite are also reported. The study is carried out in the concentration range 0.001 M to 0.01 M. At concentration lower than 0.001 M, the behaviour of ferrofluids begins to deviate from the bulk fluid properties and as the concentration approaches 0.01 M, potential aggregation effects and saturation phenomena made the solution not to disperse as desired. The Zinc spinel ferrite is synthesized by sol-gel technique.

Moment Due to Floating Buoy in Presence of Submerged Cylindrical Plate

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Abstract. In this present work, we consider a wave Oscillating Water Column (OWC) consist of a floating buoy place above a submerged cylindrical plate in water. Evaluating the overturning moment of the buoy due to scattering of water waves on the structure. The complete study is based on the theory of linear water waves which is great significant to design the model. The significant effect of the moment due to diffraction have been presented graphically for the various parameter of the structure.

B1-0093

Study of Crystal Structure and Magnetic Properties of the double perovskite oxides Tb₂FeMnO₆ Pooja Jain ^{1,2}, N.P. Lalla ¹

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Abstract. The presence of Fe, Mn, and Tb ions in the Tb₂FeMnO₆ double perovskite lattice likely leads to intricate magnetic interactions that give rise to the observed antiferromagnetic behaviour. This property could have interesting implications for potential applications in fields such as spintronics, magneto-optics, and magnetic storage devices. Additionally, by further understanding the underlying mechanisms of these interactions, researchers may be able to design and synthesize new double perovskite materials with tailored magnetic properties for specific technological needs.

Exploring the Potential of Exascale Computing: Advancements and Implications

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Abstract. Exascale Computing is the next stage of high performance computing system where computer system can perform the operation of 10¹⁸Floating point operations per second (FLOPS). Exascale Computing systems are built to give extremely high levels of computational power, making them appropriate for demanding computational activities including data analysis, sophisticated simulations, and scientific research, machine learning any more. Due to high processing capability, ESC has various applications such as climate modeling, nuclear physics, drugs discovery, Artificial Intelligence (AI) etc. Power Management, hardware reliability, software scalability, data flow optimization, and security considerations are few challenges of Exascale Computing. This article provides an overview of operating system; development and the different applications are discussed in Exascale Computing such as genomics, drug discovery, data analysis etc. This research paper also presents advantages and difficulties in Exascale Computing.

B1-0095

Structural and Transport Properties Investigation of Cobalt and Copper-Doped Iron-Disilicide Thermoelectric Material

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Abstract. The increasing energy crisis creates a negative impact on the global environment. Thermoelectric devices offer a significant solution to the energy crisis by enabling efficient energy conversion and harnessing waste heat. The efficiency of the thermoelectric devices depends on the thermoelectric materials' transport properties, which are enhanced by the elemental doping on the materials. FeSi2, or iron disilicide, has emerged as a promising thermoelectric material with unique properties that make it a subject of considerable research interest. Its stability and non-oxidant properties make it suitable for high-temperature applications. This study discusses optimising and exploring double-doped (Cobalt and Copper) semiconducting FeSi2 materials. The arc melting in the argon atmosphere followed by spark plasma sintering at 1273 K for 5 minutes holding with 50 MPa pressure and 48 hr. subsequent heat treatment at 1173 K are used as optimised parameters and investigate the effect on the thermoelectric properties of iron di-silicide with double doping. The effective doping of Cobalt on the Fe site and copper doping at the Si site significantly enhances the electrical conductivity as well as the Seebeck coefficient, which leads to an enhancement in the power factor, and the double doping results in a negative Seebeck coefficient value, which confirms the ntype semiconducting nature. The thermoelectric properties are showing an increasing trend with the increase in the temperature with the cycle of 300 K to 873 K.

Synthesis and Characterization of ZnO added Higher Manganese Silicide Thermoelectric material

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Abstract. In environmentally friendly and sustainable energy sources, thermoelectric energy production is now recognized as a scientifically promising technique. Thermoelectric technology is a very efficient method of converting thermal energy into electrical energy, enabling the utilization of diverse heat sources such as waste heat generated by industrial operations, solar radiation, and even the human body. TEGs offer the effective utilization of heat sources, sustainability, varied applications, durability, no maintenance and zero net emissions. However, the challenges include non-toxic materials usage, low material efficiency, and high production costs. Currently, thermoelectric materials used in thermoelectric generators (TEGs) consist of expensive compounds and pose potential hazards. There exists a necessity within the field of thermoelectric research to explore alternative approaches and formulate novel guiding concepts. Higher manganese silicide (HMS) emerges as a highly potential thermoelectric material comprising economically viable and environmentally friendly constituent elements. Furthermore, the power generation efficiency of higher manganese silicide will drive considerable potential for energy generation applications. But, to enhance the figure of merit, we endeavoured to include nanostructured ZnO into a higher manganese silicide using advanced synthesis methods and techniques. The crystalline structures of these entities undergo a thorough examination, focusing on meticulously analyzing their morphological aspects and carefully evaluating their thermoelectric transport capabilities.

B1-0097

Anode Materials in Lithium Ion Batteries

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Abstract. As the world is moving towards technological advancement and industrial revolution, the need for eco-friendly and portable energy sources for various applications is and will going to increase. We are surrounded by so many gadgets to run our daily life smoothly. Li-ion battery stood out as the most reliable and suitable device for storing energy so far which have applications from small scale to bigger applications like electric vehicles. Highest theoretical capacity of 3860 mAhg⁻¹ for Li metal anodes, lightweight, high energy density and many other parameters makes it attractive choice for the applications whereas it shows the lowest electrochemical potential of -3.04V versus standard hydrogen electrode (SHE). Researchers are now in finding the alternate materials for cathode and anode where different structural cathode materials are being tested and various anode chemistries have been tried. Silicon anode has the potential to replace the regular graphite anode-material as it has 10 times the specific capacity as compare to graphite. This paper reviews the anode materials which are currently under research to enhance the characteristics of Li-ion battery in comparison with the currently commercialized graphite anode (372 mAhg⁻¹) that how structural and morphological modification can change the properties like cycle life, shelf life, specific capacity, charge rate and stability of the materials.

Understanding the behavior of 5, 10, 15, 20-tetrakis (4 -hydroxyphenyl) porphyrin and its cation in Methanol: insights from electronic structure calculations

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Abstract. This research investigates the solvation dynamics and interactions of neutral 5,10,15,20-tetrakis(4-hydroxyphenyl) porphyrin (TPPH) and its cationic form (TPPH²⁺) with methanol as the solvent. HOMO-LUMO analysis and Global Chemical Reactive Descriptors (GCRD) results were reported using DFT method with BP86 functional. The study reveals contrasting charge transfer behaviors: neutral TPPH demonstrates an enhanced charge transfer rate upon dissolution in methanol, while cationic TPPH exhibits a reverse trend. This solvation-induced reduction in energy gap presents a potential avenue for optimizing optoelectronic devices like light-emitting diodes and laser diodes. These findings elucidate the intricate interplay between porphyrin derivatives and solvents, offering valuable insights for tailored applications across diverse scientific and technological fields.

B1-0099

Effects of GeS2 in Ge2Sb2Te5 for Phase Change Memory

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Abstract. Phase Change Memory (PCM) is an emerging non-volatile memory which can fulfil the gap between the NAND, HDD (non-volatile, high access time and low cost) and SRAM, DRAM (volatile, low access time and high cost). PCM consists of chalcogenide material sandwiched between top and bottom electrodes, insulator, and heater. Chalcogenide materials compose of one of the group VI A elements (S, Se or Te) except Oxygen with other elements of the periodic table. The most promising material of the pseudo binary tie line of the ternary system of Ge-Sb-Te is Ge2Sb2Te5 (GST) which is scalable (~ 20 nm node), high enduring ($\sim 10^5$), good electrical and optical contrast ($\sim 10^4$), easily switchable (in ns) between amorphous to crystalline phases. There are many phase change properties which can be improved by doping elements/compounds which shouldn't change the basic lattice structure of the GST. In order to improve thermal stability, ten years data retention and SET-RESET current, GeS2 has been doped in Ge2Sb2Te5 and deposited of about 100 nm thin films of (Ge2Sb2Te5)1-x(GeS2)x where x = 0, 0.05, 0.10, 0.15, 0.20, 0.25 by thermal evaporation. Their structural, electrical, optical, and switching properties were investigated through X-Ray Diffraction (XRD), Resistance versus Temperature (R-T), Near infrared (NIR) spectroscopy and Current versus Voltage (I-V) measurement. Ten years data retention and activation energies of all the films were also calculated through Arrhenius plot. An increment is observed in activation energies of (Ge2Sb2Te5)1x(GeS2)x thin films which leads to improve the life time of PCM. (Ge2Sb2Te5)1-x(GeS2)x reveal similar structure (NaCl + HEX) at metastable state. R-T curves show the better electrical contrast of about 10⁵ which can improve the ON/OFF ratio and thermal stability, widen band gap in all the films and in x=0.25 it is 0.832eV which enhanced the localization of charge carriers in trap state, and can improve the SET-RESET transitions, and higher threshold voltage with minimum current observed in all the doped films. Higher threshold voltage which is 7.24V for a lower current of 0.33mA has been observed in the (Ge2Sb2Te5)0.75(GeS2)0.25 film, and which can enhance the switching speed of PCM.

Thermodynamic Analysis of Topological Insulator LaPtBi

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Abstract. The structural, electronic and thermodynamic properties of cubic LaPtBi have been explored. The study is carried out by the FP-LAPW method employed in density functional theory (DFT). To test the structural stability, GGA schemes have been employed that predicts the stable nature for GGA calculation. The ground-state properties like lattice parameter, unit cell volume, and bulk modulus and pressure derivative of bulk modulus are computed. The computed GGA lattice parameters are in good agreement with available experimental data. Band structure displays their topological insulator nature. Finally, the investigation of diverse thermodynamic quantities has also been conducted under high pressure and temperature. Thermodynamic properties are reported for the first time.

B1-0101

Structural Phase Transition of S doped Ge-Te Thin Film for Phase Change Memory

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Abstract. The idea of switching property was first given by Ovshinsky in 1968, which was further used by Panasonic corporation with capacity of 500 Mb in 1990s, and commercialized by Micron, and Intel in 2018 as in 'Optane' memory. But there are some limitations like switching speed, data retention, thermal stability etc. Many researchers are working to improve the properties of phase change memory so that it can be commercialized at low cost and fast access time. One of the popular materials for non-volatile phase change memory devices is Ge-Te due to its low power consumption, compatible scalability, high switching speed, and good data retention. S doped Ge-Te films were deposited and their phase change memory properties were investigated using X-ray diffraction (XRD) characterizations, current-voltage (I-V), and resistance-temperature (R-T) measurements. From the I-V curves, a decrease in the SET current is observed in the S doped film while its R-T curve showed a significant increase in the SET resistance. This study shows an increase in the phase change memory properties by doping with S atom.

Synthesis and characterization of polycrystalline Co doped TiSe₂

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Abstract. We report the synthesis and characterization of bulk polycrystalline Co doped TiSe₂, by a self-flux method. The TiSe2 belongs to group IV-B in a class of transition metal dichalcogenides (TMDCs) that has received considerable attention due to its unique electronic, optical, and structural properties, which shows charge density wave (CDW) feature near to temperature of 200 K. A typical CDW behaviour in the ρ -T measurements with cooling and warming both. Due to the small band gap or overlapping of bands in TiSe₂, it is not surprising that addition of other elements (such as- Pd, Cu etc.) and growth conditions can affect the transport properties of TiSe2. The polycrystalline nature of Co doped TiSe₂, is characterized by powder X-ray diffraction (PXRD), which is shown in the main panel of fig. 1. The observed PXRD peaks match clearly to that of TiSe₂ and are similar to previous results. The field emission scanning electron microscopy (FESEM), is used for structural and microstructural characterization of Co doped TiSe2, which shows the layered growths with multiple planes for Co doped TiSe₂. The SEM image shown in inset of fig. 1, which shows the presence of grains, which are separated by grain boundaries confirming polycrystalline nature of synthesized sample. Also, energy dispersive X-ray spectroscopy (EDX) shown in the main panel of fig. 1, gives the elemental composition of Co, Ti and Se in approximate atomic ratio of 33%, 2% and 65% respectively for the synthesized polycrystalline sample Co_{0.03}TiSe₂. The analysis of vibrational modes of Co doped TiSe₂ by Raman spectroscopy, resulting in the occurrence of both A_{1g} and E_g modes shown in the fig. 1. Our future aim is to analyze the CDW features with different doping of Co material and magneto transport measurements.

B1-0103

Morphological Study of Calotropis Procera Fiber Reinforced Noval Phenol Formaldehyde Composite

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Abstract. Cellulose is a plentiful renewable resource that may be used to produce cellulose fibers reinforced polymer composite with a wide range of industrial uses. Natural fibers made from cellulosic material are advantageous for composites since they are biodegradable and not harmful for the environment. There is a significant number of Calotropis Procera (Aak) in western Rajasthan, India. In this work, composites are made using phenol-formaldehyde and cellulosic fiber from Calotropis Procera (Aak). Cellulosic fibers were included in the mixture at varying ratios (5 wt%, 10 wt%, 15 wt%, and 20 wt%) to strengthen the formation of Phenol Formaldehyde Resin Composites. The surface morphology of a fiber-loaded composite has been examined using a scanning electron microscope (SEM). The outcomes demonstrated that the fibers are evenly distributed in Phenol formaldehyde resin and with increasing amount of fiber amount, boding of fibers with resin is affected.

Ab Initio Study of Structural and Magnetic Properties of Co Doped ZnO Bulk

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Abstract. In this study, we investigate the electronic and magnetic properties of Co-doped zinc oxide (ZnO) bulk materials using density functional theory (DFT) calculations. The substitution of Co atoms into the ZnO lattice is systematically explored to understand its impact on the electronic band structure, magnetic moments, and stability of the material. Our calculations reveal that Co doping introduces localized magnetic moments of 3.073 μB associated with Co atoms. The electronic band structure exhibits the half-metallic nature after the Co doping with a majority spin (↑) and a minority spin (↓) magnetic configuration hybridization between Co 3d and O 2p orbitals, indicating the potential for spin-polarized transport in Co-doped ZnO. Additionally, we analyzed the formation energies to assess the thermodynamic stability. The binding energy per atom slightly decreased to -3.563 eV, indicating stable Co incorporation. These results provide valuable insights into the manipulation of electronic and magnetic properties in ZnO-based materials through controlled doping strategies.

An Investigation on Optical Properties of CdZnTe Substrate by Laser Irradiation

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Abstract: Cadmium Zinc Telluride (Cd_{0.96}Zn_{0.04}Te) single crystals grown by Vertical Bridgman technique possess good structural quality and low defect density. Such CdZnTe crystals can be used as substrate to find applications in fabricating Infrared (IR) detectors. In this paper we discuss results obtained on effect of laser (~532nm) exposure on the Raman and Photoluminescence (PL) spectrum over polished and annealed CdZnTe substrates. The incident laser power causes the increase in Raman signal of Tellurium in CdZnTe substrate and PL emission diminishes due to the burning of semiconducting material. After laser exposure of 3 mW due to localized heating only Te element left at the laser exposure area, therefore prominent Raman modes A1 (122 cm⁻¹) and E1 (142 cm⁻¹) appeared in the sample. Raman and PL mapping confirms the formation of Te-Te bond near the laser exposure area at the CdZnTe substrate.

C1-0002

Grain Size Variation On Dielectric Properties Of Gluten Free Grains At Microwave Frequency

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Abstract. Dielectric constant (ε') and dielectric loss (ε") of gluten free grains viz., finger millet, amaranth and buckwheat were measured at room temperature (22°C) at frequency 9.76GHz by using Two point method. Microwaves were employed for investigating grain size dependence of dielectric properties of the samples at three different grain size (90-150 microns, 250-300 microns and 355-425 microns). The results showed that dielectric constant of Gluten free grains increase with increase in grain size and dielectric loss also vary with grain size. This work can be an effective guide in designing a new microwave process of gluten free grains in the future.

Investigation of Dielectric parameters of Bi₂Te_{2.9}Se_{0.1} pallet

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Abstract: Topological insulator pallet of Bi2Te2.9Se0.1 has been prepared using Palletizer. Compressed Pellet into a circular (Bulk) in a shape has used for dielectric parameter study. The dielectric parameters were examined by solid test fixer of VNA at room temperature. Key words: Bismuth telluride, Selenium doping, dielectric parameters, Semiconductor.

C1-0005

Anisotropic Low Effective Mass in $p - Sn_{1-x}Eu_xTe$

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Abstract. In this study, we explore the properties of $p - Sn_{1-x}Eu_xTe$ with a focus on band dispersion and effective mass, utilizing a framework involving the \vec{k} . $\vec{\pi}$ model. We calculate these characteristics at a temperature of T=300K, using a simulated energy band gap that depends on the concentration of Europium impurity x. The energy dispersion is found to exhibit a non-parabolic behaviour, following a 4th order polynomial in k. To incorporate various interactions and effects, we derive an equation of motion under the representation of effective mass, considering the presence of spin-orbit interaction, an external magnetic field, and a magnetic impurity. The perturbation approach with $\vec{k} \cdot \vec{\pi}$ is used to account for the hybridized exchange interaction between the magnetic impurity and the carrier, as well as that between the external magnetic field and the carrier. Before and after the band inversion points at x=0.020, we extensively study the effective mass and its anisotropy, considering the experimentally simulated band gap. Furthermore, we analyze the behaviour of the effective mass of $p - Sn_{1-x}Eu_xTe$ concerning carrier concentration and the concentration of Eu impurity at T=300K. Our findings reveal remarkably low values for the effective mass, specifically m=0.006m₀, where m0 represents the free electron mass, for $p - Sn_{1-x}Eu_xTe$. This value is nearly 1/100th of the reported effective mass in a similar system, $Pb_{1-x}Eu_xTe$. This observation holds significant potential for spin-based devices like spin-Field Effect Transistors, as the much lower effective mass results in higher carrier mobility, which is highly desirable for such applications.

High Frequency Acoustic Attenuations in Dielectric Crystals

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Abstract. High frequency acoustic attenuations have been calculated for dielectric crystals of Potassium Halides (KCl, KBr and KI) for a wide range of temperature from 100-500 K. Second order and Third order elastic constants of these dielectric crystals are used to obtain the temperature dependent values of longitudinal wave velocity (V_L), shear wave velocity (V_S), non-linearity parameter D_L and D_S , thermal relaxation time τ , energy density E_0 , and using them the attenuation coefficients are calculated. Attenuation in dielectric crystal is found to be temperature dependent. Attenuation of high frequency acoustic waves is found to have maximum value for KI crystal and minimum value for KCl crystal, while, for KBr crystal it is intermediate between the above two values. Phonon-Phonon interaction is the most prominent cause of the acoustic attenuation of the high frequency waves propagating through the crystals. Shear waves are more attenuated as compared to longitudinal waves.

C1-0007

First Principle study of Electronic and Optical properties of lead-free double perovskites $ABiCuX_6$ [A = Rb₂, X = I, Br] Using Modified Becke Jhonson Potential Study

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Abstract. Lead-free double perovskites are of great interest to photovoltaic's and optoelectronics, since they are free of the toxicity and instability problems associated with lead-containing perovskites. For this study, ABiCuX6 [A = Rb₂, X = I, Br] compounds were investigated using TB-mBJ semi local (Tran-Blaha modified Becke-Johnson) potential approximation method, to predict their electronic and optical properties using WIEN2k code. According to the density of states (DOS) analysis, ABiCuX6 compounds exhibit tunable band gap properties which make them suitable for some devices such as light emitting diodes. Moreover, the materials have a high dielectric constant, a high absorption capability, high optical conductivity, and low reflectivity, which suggest they could be used in a variety of optoelectronic devices, including solar cells. Additionally, we predict that the double perovskite ABiCuX6 is the best candidate for photovoltaic's and optoelectronics applications because it has superior optical and electronic properties.

Impact of Material Used in Copper Doped Zinc Oxide Particles by Sol Gel Method

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Abstract. The aim of work showed was impact of material used and conditions in doping of ZnO via sol gel method. In this work, Copper (Cu) was doped in high amount, in ZnO via sol gel method. The structural characterizations were investigated via X-Ray Diffraction (XRD), FT-IR Spectroscopy, UV Spectroscopy. Effects on particle formations and functional bonds formed were disscussed. Dissolvent used was Nitric Acid, so prepared powder was acidic in nature, to neutralize it NaOH was added. Two types of materials was characterized to find difference in crystallite size and presence of compounds. Also displayed effect of different temerature conditions in drying via FT-IR. Crystallite size observed by X-Ray Diffraction was in range of 30nm to 150nm. Presence of Zincite, Nitratine compounds, Copper oxide were observed via peak. FT-IR peaks confirmed presence of O-H, C=C, C-N, C-H, ketones, amides functional groups in formed materials. UV-visible spectroscopy showed difference in peak absorption value, 308nm in acidic sample and 356 in neutral. The material formed via this work may be effective in agriculture industry.

C1-0009

Modified Electrical Properties and Transport Mechanism of Au/SnO₂/n- type InP Heterojunction (HJ) in the Temperature Range of 200-400 K

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Abstract. The temperature-dependent electrical properties and carrier transport mechanisms of Au/SnO₂/n-type InP heterojunction (HJ) diodes have been investigated by current-voltage (I-V) measurements. The barrier height (Φ_B) and ideality factor (n) values determined for the HJ diode changed from 0.51 eV and 4.32 at 200 K to 0.81 eV and 1.63 at 400 K, respectively. The experimental results reveal that the barrier height (I-V) increases, whereas the ideality factor decreases with increasing temperature. Using the device junction resistance (R_i) versus bias voltage (V), series resistance ($R_{\rm S}$) and shunt resistance ($R_{\rm sh}$) are derived for the Au/SnO₂/n-type InP HJ diode at different temperatures. The $R_{\rm S}$ and $R_{\rm sh}$ values of the HJ are determined in the range from 1000.5 k Ω at 200 K to $4.30 \text{ k}\Omega$ at 400 K, and $3174.6 \text{ M}\Omega$ to $0.10 \text{ M}\Omega$, respectively. The estimated R_S and R_{sh} values decrease with increasing temperature. Cheung's method is used for the determination of electrical parameters, namely barrier height (Φ_B) , ideality factor (n), and series resistance (R_S) in the non-linear region of the I-V curve of the HJ diode. The Φ_B values derived from the *I-V* method are nearly similar, indicating the techniques employed here have constancy and efficiency. The series resistance (R_S) and ideality factor (n) values derived from various temperatures are in the range from $1874.84 \text{ k}\Omega$ and 6.36 at 200 K to 12.06 k Ω and 1.98 at 400 K. The increase of R_S with the decreasing temperature may be due to the factors accountable for the increases in ideality factor and lack of free carrier concentration at low temperatures. The reverse leakage current of the heterojunction (HJ) is influenced by the Poole-Frenkel emission in the low voltage range, whereas Schottky emission predominates in the high voltage range across all temperatures.

Electrical Properties of Au/Er₂O₃/n-GaN MIS Diode with a Erbium Oxide Insulating Layer

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Abstract. The present study focuses on the fabrication of a metal/insulator/semiconductor (MIS) diode, specifically an Au/Er₂O₃/n-GaN diode using the e-beam evaporation process with a high-k rare earth oxide (Er₂O₃) interlayer. The current-voltage (I-V) characteristics of the MIS diode were investigated to examine its electrical properties and these findings were compared with the results of the Au/n-GaN Schottky diode (SD). Based on the current-voltage (I-V) characteristics, it can be shown that the MIS diode has superior rectification properties compared to the SD. The leakage current in the MIS diode is much smaller than that of the SD, with a difference of two orders of magnitude. The barrier height (BH) and ideality factor (n) obtained from the I-V characteristics are 0.79 eV and 2.43 for the SD, and 0.85 eV and 1.86 for the MIS diode, respectively. The introduction of an Er₂O₃ layer between the Au electrode and the n-GaN substrate results in an increase in barrier height and a decrease in leakage current. Cheung's and Norde's approaches are used for the determination of electrical parameters namely BH, n, and R_S in the non-linear and entire forward bias of the I-V curve. The BH values obtained from the I-V, Cheung's, and Norde techniques exhibit a high degree of concordance, indicating the reliability and efficacy of the methods applied in this investigation. 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 Er₂O₃ layer, resulting in a decrease in N_{SS}. To explore the reverse current conduction mechanism, a plot of $ln(I_R)$ against the square root of voltage (V) is drawn for both SD and MIS diodes. Under reverse bias, the Poole-Frenkel emission is the dominant current conduction mechanism for both the SD and the MIS diode.

C1-0011

To Study Electrical Properties Of Synthesized Ag_xCdS_{1-x}Thin Films With Temperature

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Abstract. The AgxCdS1-x (x = 0.00, 0.01, 0.05) semiconductor thin films are synthesized by spin coating method. Thin films were annealed in high vacuum furnace with 100° C, 200° C and 400° C temperature in presence of inert gas. Thin films were characterized by SDA with probe station on room temperature. The D.C. electrical resistance of synthesized thin films was analyzed. The composition of Ag increases in CdS with different ratio, thin films varies the order of resistance between 10^8 - 10^3 ohms with different temperature. The electrical properties of those samples change due to phase transition. The resistivity of thin films decreases with increases concentration of metal percent at particular temperature.

Study of molecular interaction and prediction of dielectric constant, refractive index, viscosity in binary liquid mixtures (1-Propanol + Benzonitrile)

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Abstract. Present work is part of our ongoing study of concentration dependent dielectric and physicochemical analysis of some nitriles with alcohols. In continuation to this we report experimentally determined values of static dielectric constant ($\epsilon 0$), optical dielectric constant ($\epsilon \infty$), density (ρ) and viscosity (η) of binary mixtures of 1-Propanol (1-PN) with Benzonitrile over varying concentration of both mixture composition in the range ($0.0 \rightarrow 1.0$) at constant temperature 303 K. The experimentally determined values static dielectric constant ($\epsilon 0$), optical dielectric constant ($\epsilon \infty$) and density (ρ) are used to compute mutual correlation factor (gab), molar polarization (Pm) and excess Helmholtz free energy (ΔG) in the mixtures. The variation of this parameters has been used to discuss type, strength and nature of intermolecular interactions between constituent species. Excess values of all determined parameters have been fitted to Redlich-Kister Polynomial and the corresponding standard deviation has been calculated. Several theoretical mixing models for static dielectric constant ($\epsilon 0$), Refractive index ($\epsilon 0$) and Viscosity ($\epsilon 0$) for the binary mixtures have been applied and their validity have been tested. Such comparison of theoretically and experimentally derived results provides better understanding about the validity of the various empirical, semi empirical and statistical theories.

C1-0013

Structural, Chemical and Electrical Properties of Au/CoPc/undoped-InP Metal/Polymer/Semiconductor (MPS)Structure

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Abstract. The present work reviews the structural, chemical and electrical properties of Au/undoped-InP Schottky diode (SD) and Au/CoPc/undoped-InP metal/polymer/semiconductor (MPS) structure are investigated using current-voltage (I-V) method at room temperature. The chemical properties of the MPS structure are investigated by X-ray photoelectron spectroscopy. The surface morphology properties are investigated by atomic force microscopy. The surface roughness of CoPc film is fairly smooth with a root-mean-square of 4.499 nm. The barrier height (BH) and ideality factor (n) values of SD and MPS are found to be 0.66 eV (I-V), 1.58 and 0.77 eV (I-V), 1.42, respectively. The MPS structure exhibited low reverse leakage current and high barrier height compared to the Schottky diode (SD). The R_S and R_{sh} values are calculated from the junction resistance and bias voltage plot, where the lower section represents the R_s in the forward bias and its highest peak represents the R_{sh} in the reverse bias. The R_S and R_S and R_S are estimated to be 3.2 k Ω and 120.7 k Ω , and 9.8 k Ω and 34.1 $M\Omega$ for the MPS diode, respectively. The barrier height (BH), ideality factor (n) and series resistance (R_S) are attained using Cheung's function. From the plot of dV/d(lnI) versus V, the R_S and n values are calculated as 1.674 k Ω and 1.79 for SD and 3.54 M Ω and 3.13 for MPS structure, respectively. Using the plot of H(I) versus V, the R_S and BH values are determined to be 1.608 k Ω and 0.69 eV for the SD, and 3.49 M Ω and 0.73 eV for the MPS diode, respectively. Achieved experimental results reveal that both the R_S values obtained from Cheung's function are in good concurrence with each other, suggesting their consistency and validity. These exploration results establish that the CoPc polymer layer is the potential for use in organic-inorganic devices.

Exploring Laser and Infrared Sensing Properties of Quaternary GeInSeS Crystals

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Abstract. The present study investigates the laser sensing and infrared (IR) sensing properties of quaternary GeInSeS crystals, synthesized through the direct vapor transport (DVT) technique. Comprehensive characterization was performed using an array of techniques, unveiling a promising candidate for versatile sensing devices. The crystals morphological attributes were unveiled through scanning electron microscopy (SEM), while energy dispersive X-ray analysis (EDAX) provided insight into their chemical composition. X-ray diffraction (XRD) confirmed the hexagonal crystal structure, laying the foundation for subsequent analyses. Furthermore, the crystals exhibited direct band gap energy of 1.12 eV. The optical characteristics of the crystals make them noteworthy candidates for laser-based sensing systems, with potential applications in precision measurement and communication technologies. The temporal response of the crystals under pulsed IR illumination was systematically studied. The crystals exhibited rapid and controlled transient behavior, indicative of their potential for capturing dynamic IR events with high temporal resolution. Overall, the study presents a comprehensive exploration of the properties and potential applications of the quaternary GeInSeS crystals, highlighting their suitability for multi-sensing devices and other innovative technologies.

C1-0015

Investigation on Optical Property of PEG/ZnO Nanofluids: The Role of ZnO Nanomaterial Concentration for Innovative Technological Applications

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Abstract. In recent years, semiconductive nanofluids (SNFs) have garnered significant interest due to their substantial role in various industrial applications, with a particular emphasis on the field of soft condensed matter technologies. SNFs have demonstrated their importance in enhancing heat transfer, enabling energy harvesting, facilitating electrical insulation and energy storage, and contributing to the advancement of diverse optoelectronic devices and controllable systems. Currently, green nanofluids have become a central point for researchers, driven by their potential to address environmental safety concerns. In this study, SNFs consisting of poly(ethylene glycol) (PEG200) as a green biocompatible base fluid (BF) with homogeneous dispersion of eco-friendly zinc oxide (ZnO) nanomaterial at ultralower to low concentrations ranging from 0.01 to 0.20 wt%, are prepared by state-of-the-art mixing and ultrasonic cavitation homogenized process. To investigate the influence of ZnO nanomaterials concentrations on the optical property of the PEG200/x (wt%) ZnO SNFs are characterized by employing advanced ultraviolet-visible (UV-Vis) spectrophotometer. A detailed analysis of the UV-Vis absorbance spectra of these SNFs, ranging from 200 to 800 nm, revealed a homogeneous dispersion of ZnO nanoparticles within PEG200. As ZnO concentration increased the dispersion exhibited tunable characteristics with dual band gaps ranging from 3 to 5 eV. This finding recognized the potential suitability of these SNFs in emerging soft technology based optoelectronic devices, photo sensors, and UV shielders.

Growth and Investigation of Thermoelectric Properties of InSbBi Crystals

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Abstract. InSb_{1-x}Bi_x (x=0,0.005,0.010,0.015) crystals are grown by vertical Bridgman technique using resistive heating furnace. The main objective of this work is to study the improvement of thermoelectric performance by different concentrations of Bismuth (Bi) in InSbBi crystals. EDAX (Energy Dispersive Analysis of X-rays) confirms that the grown crystals are pure and show the presence of In, Sb, and Bi in proportion. Powder X-ray diffractogram confirms the cubic zinc blend structure of these crystals with space group F-43m and all the diffraction peaks are matched well to the standard JCPDS-ICDD No. 6-0208. Raman spectra are recorded from 80K to 300K and Raman mapping spectra at room temperature for all above crystals have shown the presence of TO mode at 179.91cm⁻¹ and LO mode at 190.16cm⁻¹. The sharpness and intensity of Raman spectra have clearly reflected the purity and quality of the grown crystals. The electrical conductivity σ is found to increase slowly upto 450K and then increases linearly upto 600K and above that, it gets saturated in all crystals. The Seebeck coefficient remains negative showing that these crystals are n-type semiconductor and its value is found to be increased to -200 μ V/K for InSb_{0.985}Bi_{0.015} in comparison to -150 μ V/K for pure InSb near 600K. From the lattice thermal conductivity, power factor and thermoelectric figure of merit i.e. ZT calculations, it is concluded that InSb_{0.985}Bi_{0.015} at 670K gives the highest value of ZT = 0.45 in comparison to other grown crystals.

C1-0017

Temperature and Frequency-dependent Dielectric Properties of Polycrystalline ZnFe₂O₄

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Abstract. Spinel ferrites are of significant importance in various technological applications and among them zinc ferrites are of particular interest. These materials have been the subject of diverse investigations aimed at understanding the underlying mechanisms for various physical properties. The current research focuses on exploring the dielectric permittivity, ac conductivity and relaxation behaviour of polycrystalline ZnFe2O4 as a function of frequency and temperature. To achieve this, we synthesized single-phase zinc ferrite spinel using solid-state reaction. The impedance, dielectric permittivity, and conductivity of the zinc ferrite sample were studied in the frequency range of 10 Hz to 10 MHz and at temperatures ranging from 123 K to 473 K. Impedance spectroscopy study identifies the three-relaxation process. The activation energy of the one associated with grain is close to the one determined from conductivity, and their related relaxation times are thermally active, indicating that intra-grain conduction dominates as a transport mechanism. Finally, the sample has high dielectric constant over a wide frequency range making it appropriate for use in supercapacitors.

A Comparative Study of the Promising Properties of Solution Cast and Hot Pressed Treated P(VDF-HFP)/PEO-ZnO Nanocomposites

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Abstract: Advnaces in polymer nanocomposites are cruial for the dimensional design and establishment of promising performance devices. Herein, the solution cast prepared polymer nanocomposite (PNC) films composed of xP(VDF-HFP)/(100-x)PEO-2 wt% ZnO, where x varies as 20, 50, and 80 wt%, were heated up to a temperature of 90 °C and then pressed with the pressure of 2 tons and slowly cooled down to ambient temperature. The characterizations of the prepared PNC films, before and after the hot pressing treatment, are carried out by engaging advanced techniques such as UV-Vis spectroscopy, DSC, and broadband dielectric spectroscopy (20 Hz – 1 GHz). The UV-Vis spectroscopy revealed slightly augmented changes in the absorption behaviour (over the wavelength range of 800 nm - 200 nm) and also some alteration in the energy band gap of the PNCs, while the analysis of DSC thermograms infers the reduced crystallinity and thermal stability of PNC films after hot pressing treatment. The broadband dielectric spectroscopy performed on the PNCs at ambient temperatures revealed that the trend of dielectric permittivity (ϵ') dispersion of the PNC films is altered before and after hot pressing. The results explain that hot pressing treatment reduces slightly the ε' of a PNC as compared to the solution cast PNC while it keeps on increasing with the increase in P(VDF-HDP) amount in the host blend matrix. The experimental findings confirmed the multifunctionality of these flexible materials which could be useful for widespread emerging polymer device technologies

C1-0019

Study of Dielectric Nature of PZCT Poly-Crystalline Ceramics

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Abstract. In this work, the ceramics of stoichiometry Pb($Zr_{0.35-x}Ce_xTi_{0.65}$)O₃ (x = 0%, 5%, 10%, 15%) (PZ{C}T) have been synthesized through a high temperature solid state reaction. A rare earth element, cerium (Ce^{+4}), has been substituted by replacing zirconium (Zr) in PZT of 35/65 composition. The microstructures of samples were examined by scanning electron microscopy (SEM). All the samples have shown polar dielectric attribute, even with the substitution of Ce^{+4} ions at the Zr^{+4} site. With the introduction of Ce in PZT, the Curie temperature (T_c) value changed significantly from 434 °C to 448 °C. The modified samples have shown high tangent loss ($tan\delta$) values compared to pure PZT. At room temperature, the value of relative dielectric constant (ϵ_r) is first decreased for x = 0.05 sample, and then increased for x = 0.10, 0.15 samples. Also presented is the amount of diffusivity of samples obtained from modified Curie Weiss law.

A study on Magnetio-Electric Characterization of Ni-Doped PZT

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Abstract. This review paper provides a comprehensive analysis of the magnetic-electric characterization of nickel-doped lead zirconate titanate (Ni-doped PZT). The ME effect, which demonstrates the intriguing coupling between magnetic and electric properties, has garnered significant interest in recent years. The review encompasses various aspects related to Ni-doped PZT, including synthesis methods, characterization techniques, and factors influencing the magnetoelectric response. In the synthesis section, the paper discusses the different doping techniques employed to introduce nickel into the PZT lattice, highlighting the significance of proper doping concentration and processing parameters to optimize the magnetoelectric behaviour. Characterization techniques such as electrical, magnetic, and magnetoelectric measurements are extensively covered, providing insights into the mechanisms governing the observed coupling phenomenon. Moreover, the review delves into the factors influencing the magnetoelectric response in Ni-doped PZT, including compositional variations, domain structure, strain-mediated coupling, and interface effects. The paper examines the role of external factors such as temperature, electric field, and magnetic field on the magnetoelectric properties, shedding light on their impact. The review concludes by discussing the potential applications of Ni-doped PZT in diverse fields, including spintronics, sensors, and actuators. It also highlights the need for further research to optimize the magnetoelectric performance and explore novel fabrication techniques.

C1-0021

Solution Processed Ion-conducting Dielectric for Low Voltage and High-performance IZTO Thin Film Transistors: Experiment and TCAD Simulation

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Abstract. Li₅AlO₄ is traditionally known for its application as a solid-state electrolyte. In present work we have demonstrated the potential of Li₅AlO₄ as a gate dielectric material for metal oxide thin film transistors (TFTs) because of its remarkably high dielectric constant (k), which has been achieved by harnessing the enhanced capacitance offered by mobile lithium ions (Li+) within the dielectric film. Our innovative synthesis approach involves a cost-effective sol-gel method followed by a low-temperature annealing process. Through comprehensive experimentation and analysis, we demonstrate the outstanding performance of Li₅AlO₄ as a gate dielectric. The TFT fabricated by using IZTO as semiconductor channel layer shows high device performance at low operating voltage ($\leq 2.00 \text{ V}$) and high carrier mobility. The highest carrier mobility 4.52 cm²V⁻¹s⁻¹was obtained with Li₅AlO₄ dielectric TFT with very high on/off ratio ($\sim 1.4 \times 10^3$) with subthreshold swing ($\sim 240 \text{ mV/decade}$). We have also compare the experimental data with TCAD simulation.

Investigation of Structural Dielectric and Transport property of a New Oxygen Deficient Double Perovskite: YSrCuFeO5

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Abstract. The ability to intricately design, manipulate and develop new materials by structure-property modification at various scales has brought a paradigm shift in material processing and characterization. In the present communication we have reported the (structural, dielectric, impedance and conductivity) behaviour of a new oxygen deficient double perovskite $YSrCuFeO_5$ of the general formulae $A_nB_nO_{3n-1}$. Cost-effective mixed-oxide solid-state reaction route was employed in preparation of the ceramic compound. Room-temperature X-ray diffraction study reveals the overall phase and further analysis suggests tetragonal symmetry with lattice parameters a = 3.8318(4)Å, c = 7.6063(4)Å and volume = 111.68(Å)3. Microstructure study using scanning electron micrograph(SEM) confirms the formation of compact and homogeneously distributed grains with distinct grain boundaries with an average grain size of 1.32 µm. The crystallite size of the sample calculated from the Williamson-Hall plot is found to be 63.9 nm. To decipher the transport property of the compound frequency dependent conductivity study has been carried out in accordance with universal Jonscher power law. Non-overlapping small polaron tunnelling (NSPT) and correlated barrier hopping (CBH) conduction mechanisms are prevalent in the sample. Complex impedance spectroscopy study suggests negative temperature coefficient of resistance (NTCR) behaviour. The deviation of the impedance curves with their centres below the real abscissa confirms non-Debye type relaxation.

C1-0023

High Performance Organic Phototransistors Based On Tb³⁺ Doped LaPO₄ Nanoparticle-PMMA Composite As A Gate Dielectric

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Abstract. Lanthanide nanoparticles have emerged as an interesting class of nanoparticles owing to their excellent optical properties like up-conversion, tunable multicolor emission, strong luminescence, sharp emission bands, good photo stability. Because of this they find applications in lasers, waveguides, as fluorescent probes in biomedical imaging, optical thermometers, cancer diagnosis etc. However, the study of the dielectric properties of these nanoparticles and their integration in an MIM or OFET configuration has not been explored much till now. In this work, we have prepared composite of terbium doped lanthanum phosphate nanoparticles with the polymer PMMA. This composite of different nanoparticle's concentration was spin coated at different rpm to produce thin film. AFM studies of these thin films have shown that they have very low surface roughness. A MIM capacitive device having Al₂O₃ and the composite film as the dielectric layers was designed and the capacitance of these nanocomposites was tuned by varying the ratio of the polymer and nanoparticle. In the continuing work, we have integrated these films in an OFET configuration with pentacene as the channel material to design phototransistors. These phototransistors show high responsivity and detectivity in the UV region owing to the high absorption of UV rays by the nanoparticles. It was found that the mechanism behind these phototransistors was the photogating effect.

Synthesis, optical and dielectric properties of Gd-doped Strontium Niobate ceramics E. Sailaja^{1,2,a)} and G. Prasad¹

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Abstract. Gd doped Strontium Niobate $(Sr_{1-3x}Gd_{2x}Nb_2O_6; x = 0 \text{ to } 0.1 \text{ with step of } 0.02)$ has been synthesized by solid state reaction method. The as prepared samples are characterized by X-ray diffraction (XRD), Scanning electron microscope (SEM). The single phase formation of all these compounds is verified by XRD. SEM micrographs indicates that prepared materials has good sinterability and with homogeneous grain distribution. The optical absorption studies reveal that the activation energy varies with Gd content. The dielectric measurements were used to characterize the electrical behavior of these compounds. The real permittivity at room temperature decreases with increasing Gd doping. With increasing frequency the value of real permittivity decreases at room temperature. The observed dielectric properties are explained in terms of grain and grain boundary resistance.

C1-0025

Comparative study of dielectric properties of innovative PVDF/BaTiO₃/OMMT polymer nanocomposites prepared via solution casting and hot pressing approaches

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Abstract: Polymer nanocomposite (PNC) materials of outstanding dielectric properties are utilized to develop high capacity capacitors, sensors, and flexible electronic devices. In this work, the PNC films of semicrystalline poly(vinylidene fluoride) (PVDF) matrix dispersed with a mixer of ceramic barium titanate (BaTiO₃) nanoparticles and organo-modified montmorillonite (OMMT) nanoplatelets (i.e. PVDF/x (wt%) (BaTiO₃+OMMT)) were prepared firstly through solution casting approach, and thereafter, these films were hot pressed at 160 °C under the 2 tons of pressure using the polymer press film making unit. Dielectric measurements of both the solution cast (SC) and hot pressed (HP) PNC films were investigated by using dielectric relaxation spectroscopy (DRS) in the broadband frequency range from 20 Hz to 1 GHz, at ambient temperature. The hot pressed PNC films have significantly enhanced dielectric permittivity and ultra low dielectric losses in comparison to the respective solution casted films in the entire audio frequency range and the starting of bands of radio frequencies of applied harmonic electric field. The values of the dielectric constant of hot pressed pristine PVDF enhanced by about 20% and further enhanced by around 37% with the addition of 10 (5+5) (wt%) BaTiO₃+OMMT as compared to the respective solution casted films. Furthermore, a structural relaxation mechanism at a higher frequency of around 10 MHz was found which is associated with the PVDF chain segmental relaxation process. Improved dielectric properties demonstrated that these hot pressed PVDF/x (wt%) (BaTiO₃+OMMT) PNC films could be potential candidates for frequency tunable nanodielectrics and flexible dielectric substrate for futuristic capacitive energy storage and microelectronic devices.

Effect of Iodide/Triiodide Electrolyte Concentration on Solar Cell Parameters for Flexible DSSC Based on Eosin Yellow Dye

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Abstract. The performance of Dye sensitized Solar cells (DSSC) mainly depends on three components – dye, semiconductor material and electrolytes. The electrolyte is the most important component because it helps to regenerate the dye to return to ground state. The concentration of electrolyte mainly affects $J_{\rm sc}$, as well as the efficiency. This work presents a successful formation of bendable solar cell made by Al doped ZnO as n-type semiconductor and Eosin Yellow as dye. A potassium iodide solution with two different concentration has been used as electrolyte. ITO coated PET has been used as substrate. 0.08M Iodide electrolyte solution has been prepared by dissolving 0.127 gm Iodine (I_2) and 0.83 g Potassium Iodide (KI) in 10 mL of ethylene glycol. The cell shows highest conversion efficiency (η) of 1.92% with open-circuit voltage ($V_{\rm oc}$), 1.42 V and short-circuit current ($I_{\rm sc}$), 0.78 mA/cm². The lower concentration 0.04 M of I^-/I_3^- electrolyte in same structure shows 1.40% efficiency. The open circuit voltage and short circuit current for this case is 0.24 V and 3.12 mA/cm². Higher concentration of Iodine and triiodide electrolyte solution reduces the rate of recombination and improves the efficiency.

C1-0027

Needle flower-like ZnO-based chemiresistive sensor for efficient detection of formaldehyde vapors

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Abstract. The paper presents the development of a chemiresistive sensor for the efficient detection of formaldehyde vapors employing needle flower-like ZnO. The sensing material was prepared via a low-temperature hydrothermal process. The structural and morphological characterizations were performed using X-ray diffraction, and field emission scanning electron microscope. The device was fabricated by transferring the sensing material to the surface of the gold-based interdigitated electrodes using a micropipette. The sensing study revealed that the fabricated sensor was more sensitive and selective towards formaldehyde. A response of around 8 was observed in the presence of 75 ppm formaldehyde at 250 °C. The lowest detection limit of the sensor was calculated as 480 ppb. The sensor has a great potential to monitor formaldehyde vapors in the indoor environment.

The Structural and Optical Properties of $Al_xIn_{1-x}Sb$ Ternary Alloys R.K.Jhakal $^{1,2a)}$ and M.D.Sharma $^{1,b)}$

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Abstract. We present a theoretical investigation of the structural and optical properties of $Al_xIn_{1-x}Sb$ semiconducting alloys in zink-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 constant are calculated for $Al_xIn_{1-x}Sb$. Our results for $Al_xIn_{1-x}Sb$ (0<x<1) are predictions.

Optimization of Indium Tin Oxide-based All-Optical Switch Using Finite Element Method

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Abstract. The rapid development of optical communication systems necessitates the advancement of efficient and versatile all-optical switches. In this study, we propose an indium tin oxide (ITO)-based all-optical switch that harnesses the unique properties of this transparent conducting oxide material. The working principle of the proposed switch relies on the optical Kerr effect, where the refractive index of ITO changes by the influence of incident light. By exploiting the non-linear response of ITO to intense light pulses, we demonstrate its feasibility as a primary component in all-optical switching applications. With ITOs electric tunable ENZ effect, our proposed switch achieves an extinction ratio (ER) of 9.2 dB, insertion loss (IL) of 4.3 dB, and figure of merit (FoM) of 2.14. Our findings reveal that the ITO-based switch exhibits ultrafast response times and low energy consumption, making it suitable for high-speed optical networks.

D1-0002

Manipulation of Slow Light in Graphene's Landau Level

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Abstract. Recently, within the infrared regime, graphene materials have exhibited intriguing optical properties through their interaction with electromagnetic fields. These properties hold significant implications for various photonics applications, including optical data storage, optical communications, quantum computing, and information processing. With a distinct selection rule near the Dirac point of Landau levels, we have undertaken an investigation into the controllable behaviour of slow light within quantized four-level graphene nanostructures. We have derived the relevant equations of motion for probability amplitudes and group index by the utilization of quantum mechanical Schrödinger-Maxwell formalism along with a perturbation approach. By harnessing the phenomenon of electromagnetically induced transparency (EIT), we have achieved a remarkable enhancement of the group index (n_q) of the probe pulse, surpassing 10³ times its original value, especially under the influence of strong magnetic fields (~10 T). This enhancement can be precisely managed by manipulating factors such as the Rabi frequency of the control field, detuning, and dephasing rates from their corresponding energy levels. Furthermore, through the integration of an additional control field and appropriate magnetic fields, we can tune the group velocity of the probe, transitioning it from fast to slow light and vice versa. The outcomes of this study open avenues for new applications in graphene-based nano-electronic devices, all-optical switching, and quantum computing. This research embodies the potential for pioneering advancements in the field.

Laser Intensity Profile across a Spatial Light Modulator to Generate Aberration Free Holographic Optical Traps

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Abstract. We present a simple technique to determine the laser beam profile across a spatial light modulator (SLM) to generate structured light, in particular holographic optical traps. The algorithms for generating holographic optical traps or any pattern of light use incident laser beam profile over the active area of SLM as an input to generate the desired pattern of light. In general, the incident laser beam is assumed to be centered on the spatial area of SLM. In practice it is difficult to ensure the beam centering on the SLM with a resolution down to 10-20 µm, the pixel pitch of SLM. We present here a method to map the intensity of the laser and hence the beam center location on the SLM. The SLM is divided into many sub-sections and each subsection is optimized for the spatially varying phase response. Each of the sub sections are displayed with a blazed grating after optimization with other subsections kept blank. The power contribution is measured from each of the sub-sections to the first order diffracted spot at the Fourier plane of SLM and hence the laser beam profile. We also demonstrate the effect of different beam center locations by displacing the laser beam center to various locations on SLM in the trap generating algorithms and create a mismatch in the actual laser beam center as incident of SLM and the beam center used in algorithm. The effect of mismatch on various trap properties such as efficiency, uniformity and trap quality is studied. The power of the method lies in having mapped the laser intensity across the surface of SLM, this allows in setting up holographic optical tweezers with any arbitrary laser beam profile instead of conventional Gaussian laser beam for structured light generation.

D1-0004

A Unique Approach to Exactly Solve Optical pulses in Nonlinear Meta-materials

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Abstract. Nonlinear wave propagation in optics has led to innumerable innovations in several fields, the most notable of which is the study of fibre optics. The study of optical solitons in meta-materials is a new and exciting field of research where several theoretical and experimental results have been shown. Meta-materials have been a subject of intense theoretical and experimental investigations due to their wide range of potential applications from super-resolution to cloaking. However, they are artificially structured materials where both the electric and the magnetic responses can be obtained at any required frequency regime. Most meta-materials show linear response where the dielectric permittivity (ε) and the magnetic permeability (µ) do not depend on the electromagnetic field intensities. However, the nonlinear meta-materials can be designed by putting together an array of thin wires and split ring resonators (SRRs) into a nonlinear dielectric. There have been investigations of ultra-short pulse propagation in nonlinear NRM where a wide class of solutions for bright and dark solitons phase locked with the sources has been analyzed for distinct parameter ranges. In this article, the nonlinear pulse propagation has been analytically studied by solving the nonlinear Schrödinger's equation (NLSE) in bulk media exhibiting frequency dependent dielectric permittivity (ϵ) and magnetic permeability (μ). The exact solutions obtained are shown to be of trigonometric & localized types. The analytical and simulation based method has been further extended to investigate the intensity distribution in a nonlinear meta-material which behaves as a negative refractive medium (NRM), where both ϵ and μ are shown to be dispersive and negative in nature. It is seen that the peaks of the intensity curve decreases with increase in frequency towards the magnetic plasma frequency. The stability of the solitonic solutions has also been established.

LSPR Enhanced In-situ Ellipsometry for Heavy Metal Ions Detection Using Chitosan Probe

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Abstract. This work investigates the performance of LSPR-enhanced Ellipsometry for the selective and sensitive detection of heavy metal ions,i.e., Cu⁺⁺ and Zn⁺⁺ ions. The LSPR sensor chip comprises partially embedded Au and Ag/Au alloy nanoparticles on a glass slide. The chitosan was used as a capturing probe for the Cu⁺⁺. All the experiments were performed using our customized and user-friendly 3D-printed SPR module incorporated with a commercial ellipsometer under Total Internal Reflection (TIR) configuration.

The well-known toxic heavy metal ions include Cr⁺⁺, Pb⁺⁺, Hg⁺⁺, As⁺⁺, Cu⁺⁺, Zn⁺⁺, Cd⁺⁺, Ni⁺⁺, Co⁺⁺, Sn⁺⁺, etc.. Heavy metal ions harm aquatic life and humans if they accumulate beyond the permissible limit. The contamination of heavy metal ions is a significant problem to the environment as it causes severe risks to the ecosystem as well as to human health. Thus, developing adequate techniques for accurately detecting and removing heavy metal ions is essential. Compared to conventional techniques, implementing nanotechnology has several advantages, like lower detection limit, wide linear range, high sensitivity, and selectivity, for the detection and removal of heavy metal ions from water and food resources. Our approach is to develop a label-free, non-destructive, non-invasive, rapid optical sensing tool by integrating two highly surface-sensitive techniques-Localized Surface Plasmon Resonance (LSPR) and Ellipsometry for tracing the heavy metal ions in water media. The Ellipsometry measures the amplitude ratio and phase change of s- and p-polarized light in terms of Psi (Ψ) and Delta (Δ) parameters.

D1-0006

Fast light effect of surface modes at 1D magnetized plasma ferrite crystals

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Abstract. The dispersion of surface modes at new structure, one dimensional (1D) magnetized plasma ferrite layer is deduced by using transfer matrix method (TMM) method and employing Maxwell's equation theoretically and numerically. Wide photonic band gap and very narrow pass band is reported when partnering materials are magnetized plasma and ferrite. Manipulation of band gap properties can be performed by tailoring filling factor, plasma frequency and external magnetic field. The anomalous dispersion implies that the electromagnetic wave (EM) EM wave is propagating with superluminal or negative group velocity i.e. the EM wave appears to exit the medium before it enters. Negative group velocity can be attributed to the fast light effect in which group velocity should be antiparallel to group index and total power of modes. Such effect can be explored further to find applications in ultrafast photonics and optical delay lines.

Controlling Surface Plasmon Polariton Modes in a Metallic Slab Waveguide with a Nonlinear Medium

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Abstract. Surface plasmon polaritons (SPPs) are fascinating electromagnetic phenomena that occur at the interface between a dielectric material and a conductive medium, such as a metal. These exotic waves are a result of the strong coupling between light and collective electron oscillations, or plasmons, on the material's surface. SPPs have garnered significant attention in the fields of optics. nanophotonics, and materials science due to their unique properties and potential applications. Controlling surface plasmon polaritons (SPPs) is of paramount importance in various scientific and technological fields like subwavelength imaging, sensing, energy harvesting, optical communication, medicine etc. In this work, we theoretically investigate the possibility of controlling SPP propagating along a slab waveguide with the inclusion of a nonlinear material. The dispersion relation supported by the metalling slab waveguide is derived and solved numerically. The dependence of the SPP propagation on the controlling parameters of the nonlinear medium is explored. The field patterns of the SPP modes are obtained to study the confinement of the modes within the guiding region. The study has shown that the propagation of surface plasmon polaritons (SPPs) is indeed influenced by the nonlinear material, and this influence is contingent on the position of the soliton-like peak. When considering surface plasmon polaritons as potential signal carriers, it becomes evident that nonlinear effects could introduce diverse control capabilities within all-optical integrated circuits. This is due to the fact that slight modifications in the refractive index of the nonlinear material can influence the propagation of surface plasmons along the interface. The results suggest that the structure has the potential for practical utilization in waveguides, splitters, and all-optical switches, offering promising applications in these areas.

D1-0008

Structural and Luminescent Properties of Bulk KSrVO₄:Sm³⁺ Phosphor for Amber LED Applications

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Abstract. The structural and luminescent properties of Sm³+ doped KSrVO4 phosphor powders prepared by solid state reaction method were investigated. The products were thoroughly characterized by powder X-ray diffraction (XRD), photoluminescence spectroscopy (PL) and diffuse reflectance spectroscopy (DRS) studies. Bulk phase KSrVO4 crystallized into the orthorhombic system with *Pnma* space group. Williamson-Hall analysis was used to estimate the crystallite size and microstrain for the phosphor to be 267.69 nm and 0.123×10^{-3} rad respectively. The PL studies of the samples exhibited intense characteristic amber color emission of intra-4*f*-shell $^4G_{5/2}$ to 6H_J transitions of Sm³+. The luminescence decay curves showed second-order exponential behavior due to variable distribution of Sm³+ within the individual crystals. The DRS studies of the bulk phosphor estimated the optical band gap to be 3.48 eV for direct allowed transition. The phosphor was optimized for 1.5 mol % concentration beyond which the concentration quenching effect due to the energy transfer between Sm³+ ions took place via electric dipole-dipole interaction. The bulk phosphor may be projected to be used in amber emitting phosphor-converted near UV LEDs for display applications.

Comparative studies of diffusion coefficients of sucrose, lactose, and fructose using double exposure digital holographic interferometry (DEDHI) technique

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Abstract. This research paper presents a comprehensive comparative analysis of sucrose, fructose, and lactose diffusion behaviors in pu re distilled water at ambient temperature using the double-exposure digital holographic interferometry (DEDHI) technique. Diffusion coefficients of these common sugars were determined with high precision, revealing insights into their respective transport properties using digital interferograms. The non-invasive and label-free nature of digital holographic interferometry allows for real-time monitoring of diffusion processes, providing valuable data for applications in food science, pharmaceuticals, and biotechnology. The double-exposure digital interferograms were recorded for 0.6 N solutions with pure distilled water from 11000 s to 14700 s on a CCD chip and processed with numerical H-digital reconstruction software. It is observed that the average values of diffusion coefficient (D) of sucrose, lactose and fructose with pure distilled water are slightly different. They are increasing from lactose, sucrose, and fructose respectively 3.710 to $6.854 \times 10^{-6}~cm^2~/s$. The average D value of fructose solution is greater than lactose and sucrose, it is $6.854 \times 10^{-6}~cm^2~/s$. The results offer a deeper understanding of sugar diffusion phenomena and underscore the versatility of the holographic approach.

D1-0010

Comparative studies of Different nanocomposites with GaAs plasmonic solar cell Anjna Chetan, Sandeep Kumar*, Rajeev Kumar and Kh. S. Singh Department of Physics, D. J. College, Baraut, Baghpat, Uttar Pradesh, India-250611.

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Abstract: GaAs based plasmonic solar cells have been investigated by estimating the effective dielectric function using effective medium theory for bare GaAs and embedded with different nanocomposites (Ag, Au, Al, and Cu). By using the effective dielectric function, we have investigated different parameters like dielectric constant, generation rate and current density to know the efficacy of plasmonic solar cells. Al and Cu are found to be better choices for GaAs plasmonic solar cells with nanocomposites.

Analysis of Defect Modes in a Binary Photonic Crystal with a Defect of **Magnetized Cold Plasma**

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Abstract: By employing the well-known transfer matrix method, we plot the transmittance spectra of a 1D symmetrical defective binary PC made of Ge and SiO2 in the form of (AB)N/2D(BA)N/2 with RHP based MCP as a defect. Here, we analyze the position and corresponding transmission of the defect mode lying in the wide PBG, with variations in defect and two layers of the binary structure, respectively. With increase in the defect thickness, the defect mode position is tuned towards a low frequency and the defect mode transmission increases from defect thickness of 8 to 12 mm. With increase in the SiO2 thickness, the defect mode is shifted towards low frequency side and corresponding transmission of the defect mode decreases. Defect mode is not observed for Ge thickness up to 2 mm, if we increase its thickness above 2 mm, the width of first wide gap decreases, and it is shifted towards lower frequency. On increasing the Ge thickness, the defect mode position is shifted towards lower frequency and transmission corresponding to defect mode increases. These novel results based on variations in both defect mode frequency and transmission, by changing the thicknesses of layers and defect width, can be employed in designing tunable reflectors and optical sensors.

D1-0012

Terahertz Transmittance Characteristics of Semiconductor and Polymer Based Ternary **Photonic Crystal**

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Abstract: A ternary photonic crystal structure is considered, whose unit cell is made of Ge, Si and polymer (cellulose acetate). The transmittance characteristics for the proposed TPC are plotted in the THz region, by employing the transfer matrix method, with variations in incident angle and layer thicknesses (in microns). When we vary the incident angle, it is found that the single bandgap obtained at higher frequency is almost independent of the incident angle and such property may be useful in designing sensors and omnidirectional reflectors (ODRs). Thereafter, on increasing the thickness of the polymer layer at normal incidence, we find that the obtained single bandgap is shifted towards lower frequency side and becomes wider. If we increase the Ge layer thickness at normal incidence, the PBG becomes narrow and is shifted towards lower frequency side and after the layer thickness above $_{6\,\mu m}$, there occur two bands, which show multiband filter characteristics. Lastly, on increasing the Si layer thickness, the band show similar behavior, while these band gaps are more narrower and the first band disappears above the layer thickness of $_{6\,\mu m}$. Thus, the novel results show the applications of such ternary PC in designing ODRs, filters, sensing devices, and space communication.

Designing of Photovoltaic Concentrators Using Multiplexed Holographic Lenses Recorded in Photopolymer Film

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Abstract. The aim of this study is to increase overall acceptance angle of the photovoltaic concentrator by recording multiplexed holographic lenses on photopolymer film for reducing tracking mechanism associated with daily movement of the sun. Interference pattern of converging spherical wavefront with mutually coherent planar wavefront is being used for recording multiplexed holographic lens system.

E1-0001

Synthesis & Characterization of Structural and Optical Properties of Nickel Chloride (NiCl₂) Doped Potassium Hydrogen Phthalate (KHP) Crystal

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Abstract. A semi-organic single crystal of potassium hydrogen phthalate (KHP, K(C6H4COOH.COO)) doped with Nickel Chloride (NiCl₂) was successfully harvested at room temperature to enhance the characteristics of KHP using a slow evaporation approach. The concentration of 1 mol % of Nickel Chloride was used during the fabrication of the NiCl₂ doped KHP single crystal. Powder X-Ray diffraction (XRD), ultraviolet visible spectroscopy and FTIR analysis were used to analyze the grown single crystal. Powder XRD investigation verified an orthorhombic crystal structure and lattice parameter. Optical energy band gap and optical transparency were measured using UV-Vis spectral, FT-IR analysis and dielectric studies confirm that the crystal undergoes appreciable alteration as a result of the incorporation of dopant.

E1-0002

Studies of Structural and Optical Properties of Nickel Chloride (NiCl₂) Doped Potassium Hydrogen Phthalate (KHP) Crystal

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Abstract. A semi-organic single crystal of potassium hydrogen phthalate (KHP, K(C6H4COOH.COO)) doped with Nickel Chloride (NiCl₂) was successfully harvested at room temperature to enhance the characteristics of KHP using a slow evaporation approach. The concentration of 1 mol % of Nickel Chloride was used during the fabrication of the NiCl₂ doped KHP single crystal. Powder X-Ray diffraction (XRD), ultraviolet visible spectroscopy and FTIR analysis were used to analyze the grown single crystal. Powder XRD investigation verified an orthorhombic crystal structure and lattice parameter. Optical energy band gap and optical transparency were measured using UV-Vis spectral, FT-IR analysis and dielectric studies confirm that the crystal undergoes appreciable alteration as a result of the incorporation of dopant.

E1-0003

Analytical Study of Cr-Doped New Ferroelectric Ba₅Ti₂O₇Cl₄ Single Crystal

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Abstract. Flux method was used to synthesize Cr-doped ferroelectric Ba₅Ti₂O₇Cl₄ single crystal. XRD studies of the crystal shows orthorhombic nature of structure with single phase. In further temperature dependent dielectric properties of crystal were studied which shows that dielectric constant of Ba₅Ti₂O₇Cl₄ single crystal was maximum at 920°C. The measured dielectric loss of the crystal shows in good agreement with the dielectric studies. Two small endothermic curves appear in dielectric constant graph which shows the phase transitions confirmed by DTA curve.

E1-0004

A Detailed Analysis on the Morphological, Optical and Electrical Characteristics of PZN-PT Single Crystals

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Abstract. Relaxor ferroelectric single crystals of (1-x)Pb(Zn_{1/3}Nb_{2/3})O₃-xPbTiO₃, (PZN-PT) of two different compositions (x = 8% & 9%) were grown by high temperature self flux method. The compositions of 'x' were chosen to be near the morphotropic phase boundary. Different orientations of rhombohedral and tetragonal domains and their coexisting phases for PZN-9%PT were confirmed from the images of polarized light microscopy. The presence of domain walls and strip like structures on the surface was observed using atomic force microscope. Refractive index was found to be 2.6 and 2.57 for PZN-9%PT and PZN-8%PT crystals respectively. Temperature dependent Raman scattering studies clearly indicate the structural phase transitions from rhombohedral to tetragonal and finally to the cubic phase upon heating. Curie temperature was found to be around 452 K and 446 K PZN-9%PT and PZN-8%PT crystals respectively. Presence of Raman bands even after the phase transition in both the samples evidence that no long-range ferroelectric order is established. Ferroelectric behaviour of PZN-PT crystals was confirmed from the butterfly like C-V curves for frequencies ranging from 10 kHz to 100 kHz. It was observed that PZN-9%PT exhibits higher capacitance when compared to PZN-8%PT.

E1-0005

Relative investigation of electronic transport of PbBi₂Te₄ and SnBi₂Te₄

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Abstract. A relative investigation of electronic transport of PbBi2Te4 and SnBi2Te4 single crystal are presented here. The observed weak antilocalization (WAL) were fitted with Hikami-Larkin-Nagaoka equation to obtain the phase coherence length at different temperature and explained in terms of electron–electron (e–e) and electron–phonon (e–p) interactions. For PbBi2Te4 single crystal e–e and e–p interactions adhere to the T⁻¹ and T^{-2.68} power laws, respectively, whereas for SnBi2Te4 single crystal e-e and e-p interactions adhere to the T⁻¹ and T^{-2.8} power laws, respectively. These show the 2D conducting channels are participating in WAL effect. Investigation of the high-field beat-like Shubnikov-de Haas (SdH) oscillations uncovers the presence of topological surface states. Obtained lower effective mass from Lifshitz-Kosevich (LK) fit and higher mobility values from Dingle analysis affirm the surface origin of the SdH oscillations.

E1-0006

Effect of organic entities on the performance of Potassium Dihydrogen Phosphate (KDP) crystals

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Abstract. The 0.5mol l-cystine and 2mol oxalic acid doped in potassium dihydrogen phosphate crystals have been developed by slow evaporation method at room temperature. The structural properties of the grown crystal were analyzed by powder X-ray diffraction technique. The functional groups of grown crystal were successfully identified by means of FTIR spectral analysis. The optical transparency of the grown crystals is examined in the range of 200-900 nm using UV-visible studies. The optical transmittance is found to be 87 % of grown crystal. The energy band gap (Eg) of grown crystal was calculated 3 eV. The Kurtz-Perry test has been employed to determine the SHG efficiency and SHG efficiency of grown crystal was 0.5 % of pure KDP crystal tested by Kurtz-Perry powder technique.

E1-0007

Investigation of the structural and third order nonlinear optical properties in L-Ascorbic Acid Single Crystal on impact of Shock Waves

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Abstract. L-ascorbic acid, or vitamin C, is a critical nutrient with various physiological roles in the body. It is obtained through diet and supplementation and is essential for overall health and well-being. Along with these properties, it has demonstrated utility in the realm of nonlinear optics, primarily owing to its third-order nonlinear optical attributes. Within the domain of third-order nonlinear optics, which encompasses the nonlinear activity of substances when subjected to high-intensity laser radiation, L-Ascorbic Acid Single Crystal stands out for its distinctive and notable characteristics. In the present work, shock waves were deliberately administered to the grown crystal to scrutinize their impacts on the material's structural, optical, and third-order non-linearity characteristics. The assessment of these impacts was conducted employing a diverse array of advanced characterization methodologies, including Powder X-ray diffraction, High-Resolution X-ray diffraction, UV-Vis Spectroscopy, Photoluminescence, and Z-Scan techniques. The analysis of Powder X-ray diffraction reveals a discernible enhancement in the crystalline quality of the grown crystal following the application of shock waves in correlation with High-Resolution X-ray diffraction results. The application of shock wave treatment was observed to augment the material's third-order nonlinearity, a phenomenon corroborated by the Z-Scan measurements. The results clearly demonstrate that shock wave application enhances the crystal's structural, nonlinear optical properties, making it more suitable for nonlinear optical applications.

Material Potential of Cassava Root

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Abstract. Present work starts with a brief introduction 'Cassava' and it's material potential are; food application, gelation with other non-toxic organic/inorganic compound, electroactivity and its role in gelation development, new material using its electroactivity and potential application to that will be considered as new applications in the view of physical/material use. Complex of few natural exudates from plants will also be probed for development of new material from Cassava. Attempt will also be made to examine the effect of (i) cross linking (ii) increase in polymer chain length of the material and their derivatives on material application

F1-0002

Analysis and Evaluation of Waste Cooking Oil as Raw Material for Biodiesel Production towards sustainability

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Abstract. In recent years, biofuels have become a popular way to use renewable biomass energy due to its benefits against environmental pollution as they act as biodegradable, non-toxic and carbon neutral fuel. The biodiesel is produced from triglycerides in the presence of alcohol with catalyst through transesterification reaction. The biodiesel acts as promising alternative for fossil fuel especially when nonedible feedstocks are exploited in the production process. The waste cooking oil (WCO) is considered as cost-effective biodiesel feedstock comparing to pure vegetable oil. In the present work, biodiesel was produced from waste cooking oil (WCO) with methanol in the presence of sodium hydroxide done at college campus thereby solving the problem of waste oil disposal. The detailed spectral and quality analysis of the synthesized component has been extensively studied by UV, FT-IR and GC-MS characterization techniques to explore its biodiesel potential and purity. The objective of this study was to reduce the raw material cost and achieve a green synthesis in real sense. It paves the way for further investigation and improvement on this diesel production and commercial enhancement in the future. Our current findings focus primarily on mass fuel production process by using waste cooking oil from various sources, thereby making it a competitive alternative to commercial biodiesel production and ensure sustainability.

Exploring the Nutrient Capture Efficiency of Activated Biochar

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Abstract. Biochar has gained significant attention as a sustainable and effective soil amendment due to its potential for increasing nutrient retention and improving overall soil health. In this study we investigated the nutrient capture capacity of activated biochar surface pores for NPK (nitrogen, phosphorus and potassium) fertilizer application. Activated biochar was prepared using Ocimum basilicum wood as precursor through high temperature thermal treatment under nitrogen atmosphere. The resulting activated biochar exhibited enhanced porosity and surface area making it an ideal candidate for nutrient capture. Experiments were conducted to evaluate the capture efficiency of activated biochar for NPK nutrients. The biochar samples were exposed to simulated fertilizer solutions containing known concentration of NPK nutrients and the nutrient uptake was quantified using spectroscopic analysis techniques. Our finding demonstrates that activated biochar exhibits a high affinity for capturing NPK nutrients within its surface pores. The increased porosity and surface area provide ample binding sites for nutrient adsorption thereby reducing leaching losses and improving nutrient availability to plants. Furthermore we investigated the influence of various factors including the structural analysis (using XRD), chemical composition (using FT-IR), surface area of biochar using (iodine adsorption number (IN), thermal behaviours (using TGA) and BET surface area analysis. The results highlight the importance of optimizing these parameters to maximize the nutrient capture potential of activated biochar. The findings could contribute to the development of novel biochar based fertilizer that improve nutrient use efficiency and reduce environmental impact in agriculture.

F1-0004

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

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Abstract. Purpose- 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.

Finding- In the current research effort, surfactants used in comparative studies have been combined at the necessary concentration for the same experiment. It has been emphasised to utilise a mixed surfactant for solar energy conversion in order to increase electrical output through solar energy conversion and high solar energy storage.

Significance- 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 mechanism.

Crystallographic Study of 3-methoxy-4-(prop-2-ynyloxy)benzaldehyde using Laboratory X-ray Powder Diffraction Data and Hirshfeld Surface Analysis

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Abstract. *Ab-initio* crystal structure determination using laboratory X-ray powder diffraction data of 3-methoxy-4-(prop-2-ynyloxy)benzaldehyde (1) has been carried out. The indexing of X-ray powder diffraction pattern resulted in monoclinic unit cell. After solving the structure, the Rietveld refinement converged to $R_p = 0.0404$, $wR_p = 0.0548$ for 1. The nature of intermolecular interactions in 1 has been analyzed through Hirshfeld surface and two-dimensional fingerprint plot. The crystal packing in 1 is influenced by C-H···O bonds and π ··· π interactions, which assemble molecules into three-dimensional supramolecular framework. Hirshfeld surface analysis of 1 as well as a few related benzaldehyde derivatives retrieved from the Cambridge Structural Database (CSD) indicate that about 60% of the Hirshfeld surface areas in these compounds are due to H···H and C···H contacts.

F1-0006

One Step Combustion Synthesis route of Zn_(1-x-y)Al₂O₄ (x=Ce³⁺, y=Eu³⁺) Phosphor for Solid State Lighting

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Abstract. Zinc aluminate (ZnAl₂O₄) is a mixed oxide of aluminium and zinc and belongs to spinel group. It is widely used as catalyst, ceramic and electronic material. Several research has accomplished to incorporate rare earth and transition metal in ZnAl₂O₄ lattice for the application in display technologies. ZnAl₂O₄ was studied as host lattice for trivalent rare-earth ions such as Tb³⁺, Eu³⁺ and Dy 3+ that emit light in the visible range. It has been observed that the optical band gap of ZnAl₂O₄ is 3.8 eV, signifies the material is transparent for light possessing wavelength under ultraviolet range. Therefore, this material can be used for ultraviolet photoelectronic devices. Over past few years several research was reported based on the photoluminescence properties from X-ray photo electrons to infrared luminescence., Aluminates with Ce³⁺ doped lattice have attracted attention due to cost-effectiveness, high chemically stable, weather resistance and has variety of crystal structure. In the present study the Ce³⁺ doped ZnAl₂O₄ phosphor. Our literature survey revealed extensive spectroscopic study especially on cerium doped ZnAl₂O₄ scarcely exist in respect to the structural, morphological and photoluminescence properties. Keeping in view of this, in the present work, we have synthesized the ZnAl₂O₄ host doped with varying amounts of cerium and europium ions via combustion route. The phenomenon of concentration quenching, energy transfer from ultraviolet to red region, colour chromaticity, crystal structure and luminescence properties were investigated. This study suggests that the zinc aluminates co doped with europium and cerium is well suitable for solod state lighting.

Efficient Photocatalytic and Antibacterial Activity of Green Synthesized CoO/g-C₃N₄ Nanocomposites

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Abstract. In the present work CoO/g-C₃N₄ nanocomposites have been synthesized using fresh *Ficus religiosa* (*F. religiosa*) plant leaves in three different weight ratios, i.e., g-C₃N₄: CoO 1:1, 2:1 and 3:1 with polymerization. Here, the proposed study used a variety of analytical methods to characterize the as-prepared CoO nanoparticles and g-C₃N₄@CoO nanocomposites, including UV-Vis spectroscopy, a diffraction pattern (XRD), SEM coupled with EDX analysis and FTIR. Green synthesized g-C₃N₄/CoO nanocomposites were characterized FE-SEM and FTIR. FTIR spectra revealed the presence the functional group thereby confirming the formation of composites. FESEM analysis revealed the morphological aspects of the as-synthesized nanocomposite material. Photocatalytic activity of green synthesized g-C₃N₄/CoO nanocomposites was examined by the degradation of Methyl Orange dyes. Almost 95% of degradation efficiency was observed for MB sample. This photocatalyst is a potential visible light active material for the photocatalytic treatment of dyes in water.

F1-0008

Improved Ultra-sonochemical Synthesis of triazine based Pyrazoline derivative using different catalyst

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Abstract. Synthesis of 1-(4-(4,6-bis(4-substitutedphenylamino)-1,3,5-triazin-2-ylamino)phenyl)-3-(4-substitutedphenyl)prop-2-en-1-one (2.24) by using 1-(4-(4,6-bis(substitutedphenylamino)-1,3,5-triazin ylamino)phenyl)ethanone (2.23) with different aldehyde under ultrasonic irradiation and subsequently N2-(4-(4,5-dihydro-5-(4-substituted)-1-phenyl-1H-pyrazol-3-yl)phenyl)-N4,N6-bis(4-substituted)-1,3,5-triazine-2,4,6-triamine (2.25) are formed under ultrasonic irradiation in the presence of phenyl hydrazine and acetic acid. Standard spectrum data were used to describe the pyrazolines, which were produced in high to excellent yields (81-89%). The procedure is straightforward, and the findings show that, unlike traditional heating, ultrasonic irradiation resulted in better yields, faster reaction times (10-20 min.), Energy saver and milder conditions.

Organic Optoelectronic Transistor Based On Chitosan-AgNps Composite for Neuromorphic Visual Systems

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Abstract. Environmentally friendly and biodegradable electronics are currently drawing more and more attention. Biocompatible artificial synapses with learning capabilities are intriguing for neuromorphic applications. Chitosan has attracted a lot of interest in the study of synaptic transistors due to its non-toxicity, biocompatibility, renewability, and significant double-layer effect. However, it is challenging to use chitosan-based synaptic transistors with visible light as an external stimulus because chitosan typically absorbs in the deep ultraviolet region. We have synthesized chitosan-AgNps composite with an absorption peak of around 420 nm (in the visible range). Here, optoelectronic synaptic transistors based on chitosan-AgNps composite are made on a glass substrate using the solution process method. When a 375 nm light pulse was illuminated, typical synaptic properties including excitatory postsynaptic current, paired-pulse facilitation, frequency-dependent characteristics, and long-term plasticity were successfully mimicked. Our results demonstrate optoelectronic chitosan-AgNps composite-based transistors that mimic the biological synaptic behavior.

F1-0010

Photogalvanic cell with natural Surfactant (Acacia Concinna): Enhancement of storage capacity of cell

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Abstract. Several dye-reductant combinations have been experimentally studied in PG cells in the presence of various synthetic surfactants. In this research work, for the first time the Photogalvanic effect has been studied in the presence of Natural Surfactant. The photocurrents and photovoltages in various Photogalvanic cells, containing a dye -Alizarin Red-S. reducing agents- Galactose and Natural Surfactant- Acacia Concinna, were observed. The electrical parameters have been studies in alkalines (NaOH) medium with and without Al(OH)₃ solution. In presence of natural surfactant Acacia Concinna and Al(OH)₃, PG systems have been showed drastically enhancements in storage capacity. The observed optimum cell parameters in terms of photopotential, Open-Circuits Potential, Maximum Current, Short-Circuit and Storage Capacity ($t_{1/2}$) is 139mV, 314mV, 28 μ A, 6 μ A and 22 hours 10 minutes, respectively. Absorption studies were also done with these systems.

Electron Impact Ionization Cross Sections Of Sulphide Molecules

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Abstract. In this research paper, we will calculate the total ionization cross-sections of sulphide molecules by electron impact from threshold energy to 10 Mev. The ionization cross-sections is calculated by using a semi-empirical approach. This semi-empirical approach is based on Jain & Khare formalism. In our research work, we expanded the semi-empirical approach and got the good agreement of results as we compared to the previous ones wherever available.

F-0012

Investigation of Heterocyclic Compound: Indole-3-Carbinol (I3C) Using Dielectric Spectroscopy

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Abstract. The present work aims at the investigation of dielectric properties, of Indole-3-carbinol (I3C) in DMSO over the frequency range of 10 MHz to 50 GHz. Two relaxation modes were observed for the studied system. Low-frequency relaxation mode is observed at the frequency of about 80-100 MHz, which is attributed to Indole-3 Carbinol (I3C) molecules, and high-frequency relaxation is observed at about 6-7 GHz, which is due to DMSO molecules. The structural properties of I3C have been studied through dielectric parameters such as dielectric constant (ϵ i), relaxation time (τ i), distribution parameters, dipole moment (, Kirkwood correlation factor (ϵ), and number of DMSO molecules irrotationally bound to I3C molecules (Zib), and the results have been expressed in terms of molecular interaction between solute-solute and solute solvent (I3C and DMSO) molecules.

Prosthodontic Applications of Polymethyl Methacrylate (PMMA) : BiomaterialsHemant Kumar^{1*}, Pardeep Kaur ¹

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Abstract. Polymethyl methacrylate (PMMA) is a commonly used biomaterial in prosthodontics due to its excellent biocompatibility, esthetic properties, and ease of manipulation. PMMA has been used for the fabrication of artificial teeth, denture bases, dentures, obturators, orthodontic retainers, and temporary or provisional crowns, as well as for the repair of dental prostheses. However, there is still much room for improvement and development in PMMA biomaterials. Future developments in PMMA biomaterials should focus on improving its mechanical properties, reducing polymerization shrinkage, enhancing its translucency, creating biodegradable PMMA, incorporating bioactive agents, and exploring the use of nanotechnology to create new and improved PMMA materials. With further advancements in PMMA biomaterials, it is likely that this material will continue to be an important component in the field of prosthodontics, providing high-quality, durable, and esthetically pleasing dental prostheses.

F1-0014

Assessment of Seaweed as A Potential Feedstock for Bioethanol Production: Towards sustainability

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Abstract. Bioethanol is produced from various resources of biomass, they have their own set of application and drawback, and their study is related to fermentation process. Bioethanol production from seaweed is a promising approach towards sustainability which is also cost effective and renewable. Like plants, seaweeds and algae feedstocks are also comprised of rigid cellulose-based cell walls and accumulate various complex polysaccharides, which can be hydrolyzed to sugars and subsequently be fermented to ethanol. The present investigation carried out to determine the feasibility to obtain bioethanol from a residue of seaweed, Kappaphycus Alvarezii. The bioethanol produced from the influence of some parameters on acid hydrolysis, fermentation, distillation and dehydration. Hydrolysis of spent on our sample with different concentrations of sulphuric acid (0.1%, 0.5% and 1%) was also investigated. The prepared bioethanol is tested for purity by Gas chromatography-mass spectrometry (GC-MS) characterization technique and it can be concluded that the only thing left are the methyl esters. The Seaweed biomass after extraction bio fertilizer was used as the substrate for the production of the biofuel. The ethanol was produced from seaweed, which was already used in the biofertilizer production. Many research projects have been carried out over the past few years to make commercialization more promising. The recent developments suggests that large-scale bioethanol production will be made possible in near future. Our current study showed that this method could be successfully adopted for bioethanol production from seaweed.

Fabrication and Characterization of Zinc and Nickel Incorporated Vegetable Oil-Based Bionanocomposites and Their Antifungal Activity

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Abstract. In this study, we present a novel approach for fortifying vegetable oil-based bionanocomposites with zinc (Zn) and nickel (Ni) divalent cations, synthesized through an environmentally friendly method with phthalic acid as a chain promoter. Vegetable oil-based materials are gaining prominence for their eco-friendliness, but their vulnerability to fungal deterioration restricts their practical utility. By introducing divalent metals such as Zn and Ni into these matrices, we have improved their antifungal efficacy than the virgin oil. Comprehensive characterization employing Fourier Transform Infrared (FTIR) spectroscopy, UV-Visible spectroscopy, ¹³C NMR spectroscopy and zeta sizer measurements to give physiochemical, structural and size and potential. Furthermore, our research demonstrates substantial inhibition of fungal growth and hyphal development when subjected to common fungal strains. Notably, our findings reveal that the zinc-incorporated polymer complex exhibits superior antifungal activity compared to the nickel counterpart, providing a valuable insight into the material's effectiveness against common fungal strains. This innovative approach holds immense promise for creating sustainable, environmentally friendly materials suitable for applications in packaging, construction, and agriculture. By addressing the pressing issue of fungal resistance in biodegradable materials, this research contributes significantly to the development of advanced and resilient materials tailored to meet the demands of various industries.

Synthesis of Hydroxyapatite from Bio-waste

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Abstract. The objective of the present study is to prepare hydroxyapatite from natural biogenic waste i.e., fish bone. The hydroxyapatite was prepared from fish bone with the method of heat treatment. The prepared powders were characterized by TG-DTA, XRD, FTIR and SEM-EDS, to identify the characteristic nature of the hydroxyapatite. Thermo gravimetric analysis reveals that the prepared hydroxyapatite is showing very less weight loss in the presence of heat up to 900° C. The X-ray diffraction shows the presence of hydroxyapatite phase of the synthesized powders. The Fourier transform infrared spectroscopy reveals the crystalline hydroxyapatite with the help of 560, 600 and 1036 cm-1 bands. Scanning electron microscopy shows the rod like morphology and energy dispersive X-ray spectroscopy supporting the formation of hydroxyapatite by means of Ca/P ratio.

G1-0003

Effect of MgO Addition on ZrO2-TiO2-Al₂O₃ Ternary System and sintering behavior

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Abstract. The research work is investigating of sintering behavior of ZrO2-TiO2-Al2O3 Ternary system, the composite was prepared by precipitation of hydroxides from their water soluble salts followed by calcinations and sintering, the sintering behavior studied in 1:1:1 mole ratio of ZrO2, TiO2, Al2O3 between 1550°C to 1600°C. Densification depends on the function of temperature and MgO addition. It shows in significant change in densification as well as micro-structure development upto a 1mole percentage. XRD study showed that MgO addition facilitated the stabilization of tetragonal and cubic zirconia together with aluminum-titanate and Magnesio-aluminate with a dense microstructure. This Ternary system we used to mention as composite in the proceeding orders to understand clearly and this composite (Ternary system) was used at High temperature applications, it resists to mechanical (erosion) and chemical attack and thermal properties. The role of MgO in matrix is stabilized the zirconia. The result is expected to develop the formation of MgAl2O4 spinel phase and ZrTiO4 spinel phase and produce the cubic-zirconia phase with alumina Titania reinforcement.

Effect of Crystallization Temperature on Structure Evolution, Optical and Dielectric Properties of SiO₂-Na₂O-Nb₂O₅ Niobiosilicate Glass-ceramics

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Abstract. Glass-ceramics containing orthorhombic NaNbO3 crystalline phase were successfully synthesized conventional heat-treatment of the base glass having mole percent composition 70SiO₂-15Na₂O-15Nb₂O₅ by varying the temperature. Differential scanning calorimetry (DSC) analysis carried out a heating rate of 10 K/min on the base glass revealed a high glass transition (T_g) temperature of 680°C and a sharp crystallization peak temperature at 983°C which is shifted to higher temperatures with increasing heating rate. The reduced glass transition temperature (T_{rg}) $(T_{rg} = T_g/T_m)$ has been estimated to be 0.58 and the Hruby parameter (K_H) $(K_H = T_x - T_g/T_m - T_x)$ has been found 0.7 that indicated a possibility of bulk crystallization and higher glass forming ability of the composition with good stability of the glass matrix against devitrification heat-treatment. Isoconversional model-free crystallization kinetic studies revealed a decreasing trend in activation energy with the progress of crystallization. Johsnon-Mehl-Avrami-Erofeev-Kolmogorov (JMAK) model fitting approach of conversion versus time at various temperatures of 800, 850, 870 and 900°C gave an average value of the Avrami index (n) close to 3 that points towards the predominance of bulk nucleation and growth. The critical cooling rates (R_c)(°C/s) at different transformations were calculated from the Time-Temperature-Transformation (TTT) curves between 750 to 1000°C and was observed to decrease with the increase in crystal volume fraction. Slow to medium crystallization rates were observed between 800 - 850°C and that has been increased drastically above 850°C. Interestingly, glass-ceramics with sufficient transparency containing NaNbO₃ as the major crystalline phase could be synthesized at low temperatures of 750 and 800°C with a soaking time of 30 minutes. Powder X-ray diffraction analysis of the glass-ceramic samples heat-treated for 30 mins, 2.5 and 5 h at temperatures from 750 to 900°C showed diffraction patterns corresponding to orthorhombic NaNbO3 crystal phase (JCPDS file 33-1270). The intensity and area of the diffraction peaks has been observed to increase with increase in soaking time and temperature indicating growth of crystallite sizes. Low volume fraction of NaNbO₃ grains with hexagonal morphology was observed through FESEM analysis of the glass-ceramic sample heat-treated at 750°C for 30 mins. Cylindrical morphology with spherical impingement of the grains was observed in the sample heat-treated at 750°C for 5 h. Refractive index of the base glass at 632.8 nm was found to be 1.7518 which increased to 1.7628 for sample heat-treated at 750°C for 30 mins indicated densification of the glass-ceramic upon crystallization. A non-linear third order optical susceptibility of the glass-ceramics has been increased when compared to the base glass due to progressive evolution of the non-centrosymmetric NaNbO₃ crystal phase upon ceramization. The dielectric constant (at 1 kHz) has been increased five-fold from the base glass (17.6) to the glass-ceramic samples up to 93.6 for the sample heat-treated at 850°C for 5 h. The dissipation factor has been decreased from the base glass (5.11×10^{-3}) to the glass-ceramic samples up to a minimum value of 8.79×10^{-5} .

Glass Transition Behaviour and Structural Analysis of SrCl₂ Modified Tellurite-Based Glasses Komal Poria^{a,*}, Rajesh Parmar^a, Sunil Dhankhar^b, R.S.Kundu^c

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Abstract. By using the traditional melt quenching procedure under carefully regulated atmospheric circumstances, the glass system $60 \text{ TeO}_2\text{-}(25\text{-x})\text{Bi}_2\text{O}_3\text{-}15\text{B}_2\text{O}_3\text{-x}\text{SrCl}_2$ with mole fractions x = 5, 10, 15, and 20 was created. Differential scanning calorimetry (DSC) was used to calculate the glass transition temperature (T_g), and it was shown that the T_g value increased as the amount of SrCl_2 in the glass system increased. This rise in T_g is probably due to a greater number of bridging oxygen (BO) atoms, indicating the increase in glass thermal stability. FTIR and Raman spectral data have been deconvoluted for estimating the peak, whereas each deconvoluted peak exhibits numerous peaks. The present glass system's IR and Raman spectra analysis revealed that SrCl_2 acts as a network modifier in the form of Sr-O bond. TeO_2 is made up of a variety of structural components, including TeO_3 trigonal pyramidal, TeO_4 trigonal bipyramidal, and TeO_{3+1} . BiO_6 octahedral structural units define bismuth (Bi_2O_3), which modifies networks. Both BO_3 trigonal and BO_4 tetrahedral structural units of B_2O_3 can be found in the glass system.

G1-0006

Physical and Optical Properties of Pr³⁺ Rare-Earth Ions Doped Tellurium Bismuth Borate Glasses

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Abstract. A series of undoped and Pr^{3+} doped Tellurium Bismuth Borate glasses with composition $50B_2O_3.20TeO_2.(30-X)Bi_2O_3.(X)Pr_2O_3$ (Where X=0,0.1,0.3,0.5,0.7,1 mol%) were prepared by melt quenching technique. The XRD pattern has been used to confirm the amorphous nature of all prepared glass samples, the broad hump in XRD Spectra shows the amorphous nature of the glass samples. The physical parameters like the Optical dielectric constant, Refractive index, Molar volume, Oxygen packing density, Density, mean atomic volume, rare earth ions concentration, Interatomic distance, and average molecular weight were also calculated. The dielectric constant and Refractive index both increase with the increase in dopant concentration.

Physical and Optical Properties of Pr³+ Rare-Earth Ions Doped Phosphate Glasses

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Abstract. A new series of Pr^{3+} doped phosphate glass with composition (5-x) P_2O_3 .40 Li_2O_3 .55 B_2O_3 .x Pr_2O_3 (x=0, 0.3, 0.5, 0.7 mol%) was prepared by melt quenching technique. XRD pattern of the prepared glass samples confirms the amorphous nature of glasses. The physical parameters like dielectric constant, Interatomic separation, molar refraction, and refractive index are also studied. The refractive index and dielectric constant of prepared glass increase with increased doping concentration of Pr^{3+} rare earth ions in the glass samples.

G1-0008

Structural and Optical properties of Telluroborate glasses doped with Praseodymium rare earth ion

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Abstract. The glass compositions were formulated as (50-x)B2O3·20TeO2·5Mg2CO3·15K2CO3 ·xPr6O11, with x being varied in the range of 0, 0.4, 0.5, 1, and 1.5 mol%. Using the melt quenching technique, a novel set of telluroborate glasses doped with Pr³⁺ ions has been synthesized. The structural and optical studies of telluroborate glasses doped with Pr³⁺ are reported. In the present work, the main objective is for the combined Raman, FTIR, Optical, and Fluorescence spectra of telluroborate glasses doped with Pr3+ ion to be studied. It is expected that this collective spectral study will provide further insights to better understand the doping effects of both tellurite and rare earth oxides in host glasses. All samples were found to exist in a glassy form, with a broad hump in the XRD pattern that is characteristic of an amorphous nature. The network structure of the glasses was investigated using FTIR and Raman spectroscopic techniques. The FTIR spectra reveal the various bending and stretching vibrations of the bonds within the present glass samples. The presence of various vibrational bonds of the borate and tellurite network is shown in the Raman spectra. The Judd-Ofelt $\Omega\lambda$ $(\lambda = 2,4,6)$ intensity parameters were determined using optical absorption spectra in order to explore the bonding environment around the Pr3+ ions. To unveil the radiative properties of Pr3+ doped telluroborate glass, certain significant spectroscopic parameters such as the spontaneous radiative transition probability (A), fluorescence branching ratio (β), and emission cross-section (σ e) were calculated. Among the studied glasses, higher values of σe and optical gain were exhibited by TEB0.4 glass, thereby specifying its suitability for laser applications.

Investigation Of Mechanical Properties In Ligno-Cellulosic Fiber-Reinforced Polymer Composites With Sic And Al_2O_3 Fillers

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Abstract. This study investigates the influence of fiber loading and filler content on the tensile properties of epoxy composites reinforced with a lignocellulose fiber i.e. banana fiber. Natural fiber composites have risen to popularity in engineering applications due to their ability to optimize strength, weight, and cost as the world moves toward eco-friendly materials. Banana fiber, which is derived from the pseudostems of ripe bananas, is a readily available reinforcing option. Both unfilled and filled composites containing silicon carbide (SiC) and aluminum oxide (Al2O3) are the subject of this study. Results show that unfilled composites are sensitive to fiber loading in terms of tensile strength, flexural strength, and hardness. An optimum fiber loading of 15% by weight demonstrates the highest tensile and flexural strengths. Additionally, there is a pattern whereby increasing the filler content from 0 to 20 wt. percent increases the tensile and flexural strengths, followed by a decrease at 30 wt. percent. Surprisingly, the increased flexural and tensile strengths are mostly attributable to the 20 wt.% Al2O3 concentration. This study highlights the potential for improving composite performance by tuning the fiber-to-filler ratio, a step forward in the development of environmentally friendly materials. This research adds to the growing body of evidence supporting the usage of sustainable engineering materials in today's environmentally conscious world.

G1-0010

An Emission Analysis of A Novel Trivalent Eu³⁺ Ion-Doped Zinc Phosphate Glass for Photonic Applications

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Abstract. The demand for inorganic glasses is increasing due to their diverse applications so in this study a new type of zinc phosphate glasses (ZnP) doped with Eu³⁺ ions were prepared using the conventional melt-quenching method in the following composition: $(60-x)P_2O_5$ -20ZnO-10SrO-10LiF- xEu_2O_3 , where x varied from 0.1 to 2.0%. The amorphousness of the prepared glasses was confirmed using X-ray diffraction (XRD) profiles, and the emission spectra of the prepared glasses exhibited five distinct emission bands at an excitation wavelength of 394 nm. Judd-Ofelt (JO) parameters were calculated from the emission spectra and showed a trend Ω 2> Ω 4. The radiative emission rates (A_T), stimulated emission cross-sections (σ), and quantum efficiencies (η) were also calculated. The $^5D_0 \rightarrow ^7F_2$ transition at 612 nm exhibits high intensity. The characteristic color emission of the ZnP glasses was determined by means of the Commission International de l'éclairage (CIE) 1931 chromaticity coordinates (x, y) and lies in the red region. These glasses exhibited strong red luminescence. Zinc phosphate glasses (ZnP) doped with Eu³⁺ ions have potential applications as red lighting components.

Investigations on RE-doped nanocomposite Electrolytes for Lithium Battery Applications

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Abstract. Magnesium halide and nickel halide batteries, then lithium ion batteries, ruled for several decades. Polymer batteries are the subject of the latest research, and they are of considerable scientific significance. In comparison to their liquid analogues, polymer electrolytes typically have poor ionic transmission. Consequently, numerous attempts are made to enhance its ionic conductivity by different means such as blending, adding lithium ions, plasticizers, ionic liquid, and/or inorganic additives. This study focuses on the processing and analysis of nano-polymer electrolytes made from PVC-PBMA blends for use in lithium batteries. The impact of adding rare-earth(RE) to a nano-polymer electrolyte is studied during its preparation using solution casting method. The prepared RE-PVC-PBMA blended polymer electrolytes are characterized by XRD, FTIR, ac impedance, TG/DTA, SEM, and mechanical analysis with regard to their structural characters, complex formation, ionic conductivity, thermal properties, morphological and mechanical behavior and discussed in detail.

G1-0012

Room temperature Multiferroicity and Magnetodielectric effect in (1-x) BaTiO₃-(x) CaMnO₃

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Abstract. Magnetoelectric (ME) ordering in multiferroics are technologically applicable in a variety of fields like ultra-low power and highly dense logic-memory, micro(nano) electronic, sensors, energy harvesting, actuators, spintronics, miniature antennas, terahertz emitters, electric-field controlled FM resonance, four state memories, microwave filters, feRaM, MRAM and Spintronics [1-2]. Generally, ME effects are mild and materials have low Neel temperature [3]. Most of the multiferroic materials exhibit ferroelectric and/or magnetic phase transitions at cryogenic temperatures [4]. Oxygen vacancies are important components in a material which modify the structure and properties of materials. Factors like lattice disorder get modified thereby having an effect on the electronic structure and the magnetic properties etc. As a result of such changes, more involved physical parameters like magnetoelectric coupling can be affected [5]. To investigate such changes a solid solution of (1-x) BaTiO₃-(x)CaMnO₃ (x=0, 0.03) have been investigated, in detail, using XRD, XPS, and Raman spectroscopy. The electric and magnetic properties have been investigated using dielectric spectroscopy, ferroelectric and magnetic studies. For a substitution of x = 0.03, existence of both ferroelectric and ferromagnetic nature leads to room temperature multiferroicity. The variation of dielectric properties such as capacitance, dielectric loss with applied magnetic field gives the magnetodielectric coupling, which is an indirect measure of magnetoelectric coupling. The magnetodielectric coupling is strongest in x=0.03 and has been correlated to the structural properties, changes in valence states, and oxygen vacancy (Ov). Hence (0.97)BaTiO₃–(0.03)CaMnO₃ can be used for room temperature multiferroic application.

Physical, Thermal and Optical study of bismuth modified boro-vanadate glasses: V₂O₅-B₂O₃-Bi₂O₃

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Abstract. The present study investigated the influence of varying Bi_2O_3 concentration on physical, thermal and optical properties of boro-vanadate glasses. Glasses with the composition of $60V_2O_5$ -(40-x) B_2O_3 -x Bi_2O_3 were synthesized; where x=5-25 mol% (with step of 5 mol%). The non-crystalline nature of prepared samples was confirmed with X-ray diffraction (XRD) patterns. The different properties of the processed samples were ascertained using a density measurement instrument, Differential scanning calorimeter (DSC) and ultra-violet visible spectrometry (UV-visible). The glass samples' density, molar volume, and crystalline volume increases while the band gap decreases as Bi_2O_3 content increases. The band gap was found in the range of 1.63 eV to1.92 eV. Glass transition temperature (T_g) showed a decreasing trend but increased for a sample x=20 mol%. Various other calculated parameters include refractive index (n), molar refractivity (R_m), metallization criterion (M), electronegativity (χ), optical basicity and electron polarizability (α -). The high refractive index values (2.77-2.92) and low metallization criterion (ranging from 0.286-0.310) observed across all samples indicate the potential suitability of these glasses for non-linear optical purposes.

G1-0014

FTIR and Raman spectroscopic studies on PbF2-Al2O3-Bi2O3-B2O3-CuO glasses

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Abstract. The usual melt quenching procedure was used to generate unique glass samples containing the chemicals PbF₂, Al₂O₃, Bi₂O₃, B₂O₃, and CuO. The Al₂O₃ content was increased by reducing the amount of PbF₂ in the samples. Subsequently, the produced samples underwent X-ray diffraction (XRD), Fourier-transform infrared (FTIR), and Raman spectroscopy measurements to conduct a comprehensive structural study. The X-ray diffraction spectra indicated the absence of distinct peaks, providing evidence for the amorphous nature of the materials. Fourier Transform Infrared (FTIR) spectra were obtained throughout the spectral range of 200 to 2000 cm⁻¹. The deconvoluted spectra were afterward used to precisely determine the specific locations of the infrared (IR) bands. The infrared spectra provided evidence of distinct infrared bands associated with the borate, Pb²⁺, and AlO₄ units present in the glass structure. The analysis of Raman spectra demonstrated that the presence of PbF₂ and Al₂O₃ induced modifications in the network structure of the PFABBC system in the examined glass samples.

Structural, morphological and luminescence properties of Ba₂Al₂SiO₇:Ce³⁺ Phosphors

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Abstract. Ba₂Al₂SiO₇:Ce³⁺ (BASO: Ce³⁺) phosphors for blue light emission were prepared using Combustion Synthesis Method followed by annealing at 1100° C for 12 Hours. X-ray Diffraction analysis was done to find out phase structure and lattice parameters. Fourier Transform Infrared (FTIR) spectra was recorded to identify the functional groups present in the sample. Scanning electron microscopy (SEM) was performed to get the details of Surface morphology and energy dispersive X-ray spectroscopy (EDX) was done to know the elemental composition. The XRD plots were matched well with the reference data and the tetragonal phase formation was identified. There were no additional peaks observed with the addition of dopant. Fourier Transform Infrared Spectroscopy (FTIR) was carried out to identify the presence of Ba-O, Si-O, Al-O band vibrations. The effect of the doping concentration on the luminescence properties of BASO: Ce³⁺ phosphors was investigated using photoluminescence (PL) studies. The Ce³⁺ doped BASO phosphors give blue emission when excited at 328 nm wavelength. The PL intensity was maximum for 0.2 mol% of Ce³⁺ concentration. The color coordinates of the prepared phosphors are calculated.

G1-0016

Structural and Dielectric Properties Of PVDF/CoFe2O4@BaTiO3 nanocomposites

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Abstract. Polymer nanocomposites (PNC) are gaining interest due to their flexibility and multiferroic nature. Interesting properties were observed when magneto-piezo component merged together in our work. PNC with various applications in multifunctional devices are associated with excellent Dielectric, Magnetic and Magneto-dielectric properties. The reason behind the idea of core shell PNC is to reduce its leakage current density and introduction of PVDF is to enhance its dielectric properties, reduce dielectric loss & improve flexibility in the PNC. PNC were prepared through Coprecipitation and Sono-chemical route due to its eco-friendly nature. The PNC were composed of CoFe2O4@BaTiO3 (CBT) core-shell fillers and poly (vinylidene-difluoride) (PVDF) matrix. The pellet of PVDF/CBT was synthesized in varying weight fractions i.e., 5%,10%,20%,30%,40% & 50% by novel cold pressing method. XRD ensures the pure phase of CBT & PVDF in the PNC and FTIR gave the information of various functional group attached with PNC. FESEM Micrographs are showing the spherical nanoparticles and EDX & dot mapping shows the homogeneous distribution of all elements in PNC. Dielectric measurements were carried out in frequency range of 20Hz to 2MHz at room temperature. The Dielectric studies reveal that the relaxation and conduction mechanism is associated with PNC.

Influence of MnO₂ on PbO-CdO-TeO₂-B₂O₃ glasses: Structural study

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Abstract. A set of unique glasses, consisting of the chemical composition PbO-CdO-TeO₂-B₂O₃-MnO₂, were synthesized in order to investigate the impact of MnO₂ on the physical and structural characteristics. The samples underwent analysis using X-ray diffraction (XRD), ultraviolet (UV) spectroscopy, and electron paramagnetic resonance (EPR) spectroscopy techniques at ambient temperature. The density readings exhibited an increase from 3.895 to 3.957 g/cc, which suggests that the presence of MnO₂ concentration led to the transition of BO₃ units into BO₄ units. The introduction of MnO₂ resulted in a reduction in the band gap values, while concurrently leading to an increase in the Urbach energy. The findings of this study indicate that the presence of MnO₂ in the glass structure leads to an increase in the amorphous phase. Additionally, the refractive index values were seen to rise from 2.252 to 2.279. The electron paramagnetic resonance (EPR) spectra of the aforementioned samples exhibited resonance signals at g = 4.3, g = 3.0, and g = 2.0. The resonance signal has a six-line hyperfine structure that is centred on a g-factor of 2.0. The A value of around 60 x 10^{-4} cm⁻¹ signifies the presence of covalent bonding inside the anion, while an A value of approximately 100×10^{-4} cm⁻¹ denotes the predominance of ionic bonds.

G1-0018

Radiation shielding features of PbF2-PbO-B2O3-CuO glasses using Phy-X software

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Abstract. This article examines the effect that lead fluoride on the radiation-shielding properties of lead borate glasses that contain copper ions and summarises the findings. The density of the samples was determined by using the Archimedes principle after they were created using the melt quenching procedure with the components PbF₂-PbO-B₂O₃-CuO. It was discovered that the density of the samples rose as the amount of PbF₂ rose. In order to conduct an examination of the radiation-deflecting properties of the samples, the Phy-X programme is used. Shielding characteristics such as Mass attenuation coefficient (MAC), Linear attenuation coefficient (LAC), and others were calculated with the assistance of this programme. In the low photon energy range, it was discovered that the LAC values were rather high; however, these values began to decline as the photon energy continued to decrease. Both the LAC and the MAC exhibit an absorption edge at 0.1 MeV. This edge was caused by the absorption of K-electrons from Pb atoms, and it was seen in both the LAC and the MAC. The half value layer (HVL) had a flat fluctuation in the low photon energy area, however on the higher energy side it dramatically surged to its maximum values before experiencing a minor decline. This was seen in both regions of the spectrum. The presence of PbF₂ in these glasses resulted in a reduction of the HVL values, and this reduction was more pronounced for samples with higher densities. The samples that include a greater concentration of PbF₂ will have superior characteristics in terms of shielding.

Electron Paramagnetic Resonance Studies on Mixed Alkaline Earth Oxide Borotellurite Glasses doped with Cu²⁺ and VO²⁺ Transition Metal Ions

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Abstract. Transition metal ions such as 1 mole % of CuO & 2 mole % of V₂O₅ doped in mixed alkaline earth oxide boro-telluriteglass samples were prepared. Electron paramagnetic resonance (EPR) study has been carried out to know about metal – ligand bond in the glasses. Spin-Hamiltonian parameters (g & A), bonding parameters (α^2 & β^2), Fermi contact interaction parameter (K), A_{\parallel}^{-} & A_{\perp}^{-} and line width parameter (H_P) values are evaluated. For Cu²⁺ doped glasses it is observed that $g_{\parallel} > g_{\perp} > g_e$, this is characteristic feature of d_{x2-y2} ground state. G= $(g_{\parallel} - g_e)$ / $(g_{\perp} - g_e)$ values indicates a strong exchange coupling takes place among the magnetically non- equivalent Cu²⁺ ions in unit cell. R = $(g_2 - g_3)$ / $(g_1 - g_2)$ values are less than unity, indicates the ground state of Cu²⁺ ions is ${}^2B_{1g}$ (d_{x2-y2}). For VO²⁺ doped glasses it is observed that $g_{11} < g_{\perp} < g_e$ and $A_{11} > A_{\perp}$ shows the presence of unpaired electron is d_{xy} orbital. This is a characteristic feature of tetragonally compressed complex.

G1-0020

Luminescence investigations and decay behavior of praseodymium incorporated borate glasses modified by MO (M = Ca, Ba, Sr)

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Abstract. The current study aims to investigate the impact of various alkaline earth metals on fluoride borate glass. Glasses with 0.5 mol% embedded Pr³⁺ in the borate glasses modified by MO (M = Ca, Ba, Sr) were prepared using melting and quenching techniques. The present investigation aims at elucidating the luminescence behaviour, luminescence spectra of the glasses are presented and discussed in relation to the impact of alkaline earth metals (CaO, BaO, SrO) and the luminescence lifetimes for the excited states of Pr³⁺ ions were analyzed in details. The luminescence and time decay both have interestingly affected due to the alkaline atomic size variation. The fluorescence decay spectra of Ba/Ca/Sr varied 0.5mol% praseodymium incorporated oxide glasses have been explicated, which is single exponential in nature. The resonance energy transfer mechanism responsible for non-radiative decay rates is clearly explored. A thorough investigation was done to have a better understanding, and the results have been reported.

Structural and FTIR Spectroscopic Study of Lead Doped $Se_{80-x}Te_{20}Pb_x$ (x=0, 1 and 2) Chalcogenide Glasses

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Abstract: Pb additive chalcogenide materials are becoming well-known materials in modern optoelectronics. In the present study, the Se-Te-Pb chalcogenide glasses are prepared using melt-quenching technique as well as structural analysis is done by FESEM and FTIR spectroscopy. The absence of any sharp characteristics peaks in X-ray diffraction spectra signify the amorphous nature of examined glassy compositions, which is further validated by FESEM. The Far-IR spectra of Se-Te Pb glassy alloy are obtained in the spectral range 150-1200 cm⁻¹. Influence of Pb content on the examined compositions has been deliberated with respect to their infrared spectroscopy. The FTIR analysis give an idea about different type of major bond and bonding structures present in the examined alloys. Moreover, theoretically estimated values of wavenumber are slightly less than experimentally deduced results. The far-IR spectra reveal that all possible heteropolar bonds are in accordance with the CBA and have compositional variation.

G1-0022

Effect of Fe₂O₃ content on DC Conductivity of Bismuth and Lead Borate Semiconducting Glasses

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Abstract. The heavy based metal oxide glass of series with compositions xFe₂O₃.(40-x)M.60B₂O₃ (M=Bi₂O₃ and PbO) have been prepared by the standard melt-quenching technique. The effect of temperature on DC conductivity has been measured in the temperature range 373-473K for the compositions. In this temperature range, the DC conductivity increases with increase in Fe₂O₃ content of these glasses and it was found that it increases more rapidly of lead borate glasses than bismuth borate glasses due to creating higher non-bridging oxygens comparatively. In these glass systems, it is expected that the DC conductivity may have contribution in the form of electronic conductivity due to electron hopping from the one valence state Fe²⁺ to the other valence state Fe³⁺. Non-linear behavior of the plots between logarithm of conductivity and activation energy indicating non-adiabatic polaron hopping mechanism.

Eu³⁺ doped Transparent Ba₂TiGe₂O₈ based Glass-ceramics: Crystallization, Optical and Dielectric Properties

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Abstract. Eu³⁺ doped Ba₂TiGe₂O₈ (BTGE) glass-ceramics (GCs) have been synthesized from the base glass of composition (30BaO-15TiO₂-55GeO₂+0.5Eu₂O₃) (mol %) following conventional melt-quenching and ceramization heat-treatment of the base glass. Crystallization kinetics analysis of the base glass enabled to determine the experimental heat-treatment temperature and time for controlled crystallization of the glass so that the average crystallite sizes could be controlled in the nanometer scale. Single-stage heat-treatment of the base glass at 750°C for varied duration of 3 - 12 h yielded transparent GCs. Structural analysis through XRD, TEM and FTIR confirmed evolution of the nonlinear ferroelastic Ba₂TiGe₂O₈ nanocrystals. Particle size analysis from XRD and FESEM revealed an average crystal size 20 -100 nm in the glass matrix. The optical band gap energies have been found to increase in the GCs heat-treated for 9 and 12 h up to 3.88eV. The local crystal environment around Eu³⁺ ions in the glass matrix facilitated in enhancement of the photoluminescence intensity of Eu³⁺ in the GCs as compared to the base glass. The room temperature fluorescence decay from the ⁵D₀ state of Eu³⁺ ions in all the samples exhibited a single exponential decay curve with increase in the average life time of Eu³⁺ from the base glass to the GCs. The dielectric constant increased and the dielectric loss decreased from the base glass to the GCs.

The Role of Transition Metal Oxide Interfaces in c-Si Solar Cells as Efficiency Improvers

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Abstract. Passivated transition metal oxide (TMO) interfaces have appeared as an alternative for enhancing the process of affordable crystalline silicon (c-Si) solar cells.TMO, including Titanium oxide, Zinc oxide, Niobium oxide, MoO₃, V₂O₅, etc., are investigated as having passivative properties. The selection of these materials is based on their compatibility with cost-effective and scalable deposition technique such as atomic layer deposition, thermal evaporation and solution based method. The effectiveness of passivated interface is evaluated by surface passivation velocity, minority carrier life time and surface passivation quality.TMO interfaces contribute to the development of high-performance and more economically viable solar cells. As the need for clean and renewable energy continues to grow, the optimization of passivated TMO interfaces remains an active area of research in the field of photovoltaic. In this review the challenges and opportunity in integrating passivated transition metal oxides interface with c-S, carrier transport mechanisms, material property optimization, manufacturing processes are discussed.

H1-0002

Dewetting Assisted Selforganization Of Carbonaceous Nano- particles Over Polymer Interface

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Abstract. The self-organization of thin polymeric film like polystyrene occurs mostly because of instability caused by various reasons like van der Waals interaction, heterogeneous nucleation resulting in rupture and holes in the thin film. These dewetted structures are widely used for various applications like capturing atmospheric water, enhancing the photoluminescence, in opto-electronic device fabrication like UV-photo detector and also used for self-assembly of biological moieties. While most groups working in thin-films have found that incorporation of nano-particles have led to arresting of thin-film dewetting, the recent works of the presenting author involving graphene nanoparticles over bio-compatible PS thin-films have explored how the dewetting dynamics of the underlying thin-film can be used as a template that leads to the formation of unique self-assembled nano-particle patterns at the interface between graphene and a thin polystyrene (PS) film at room temperature. When a minute amount of NP dispersed in a solvent is added on PS and spin-coated into a thin film, the concentration gradient caused by centrifugal force leads to a Marangoni flow that in conjunction with the dewetting of the underlying PS at the edges lead to a series of very interesting and self-assembled morphologies of the nano-particles. At the particle enriched zone near the center, the graphene-particles exhibit morphologies ranging from folds, wrinkles, flakes, onion-rings to blob structures depending on the aspect ratio. The graphene-particles thrown to the periphery are found to march back towards the central portion leading to the unique formation of very ordered nano-scale scratches on the PS substrate. The graphene nano-particles that end up into the confined rims in the intermediate region get twisted into nano-ribbons and dendrimers.

Local electronic structure of Sn white flower motifs on five-fold *i*-Al-Pd-Mn surface using scanning tunneling spectroscopy

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Abstract. Quasicrystals are aperiodic structures with long range ordering and their electronic stabilization is due to the existence of pseudogap at the Fermi level. In the present work, combined results of scanning tunneling microscopy/spectroscopy (STM/S) measurements establish the presence of a deeper pseudogap in the Sn white flower (SnWF) motifs compared to *i*-Al-Pd-Mn at room temperature.

H1-0004

Electronic Structure Of Antiferromagnetic Monolaver Cr Film

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Abstract. Low dimensional magnetism is attracting significant scientific attention with the advancement of spintronics in device applications. Magnetic properties of ultrathin films may dramatically be different from their bulk counterpart owing to alloying, adsorption and surface reconstruction. Ab-initio density functional theory (DFT) studies predicted a giant enhancement of magnetic moments of the 3d transition metal overlayers on non-magnetic substrates. Moreover, overlayers of the late transition metals (Fe, Co and Ni) and the early transition metals (V, Cr and Mn) placed on Cu, Ag and Pd substrates were predicted to attain FM p(1x1) and AFM c(2x2) configurations, respectively². Bulk Cr, with its nearest neighbour atomic distance 2.49Å, has bcc structure which demonstrates incommensurate spin density wave with magnetic moment 0.59 µ_B. According to DFT calculations, on lowering the dimensionality (e.g. monolayer deposition over Ag(001) substrate) Cr magnetic moments are enhanced upto 4.46µB due to 15% increment of the nearest neighbour distance. The ultra-sensitivity of Cr magnetic moments to isolation is due to its half-filled 3d orbitals. However, practical formulation of such a sustained 'two-dimensional' ordered AFM layer is hardly straightforward. The lattice parameter of Cr allows its pseudomorphic growth on Ag(001) with its <001> direction rotated 45° with respect to the substrate, demonstrating 0.3% lattice mismatch. On the other hand, the higher surface free energy of Cr (according to Bauer's criterion) preferentially stands for its multilayer growth over Ag(001). In fact, scanning tunneling microscopy (STM) studies on the same system did not support the existence of flat monolayer growth³. At low temperatures (100 K), growth takes place via the hit-and-stick (random deposition) mode, as shown experimentally. On the other hand, very high temperatures (above 500 K) result in Cr agglomeration, as well as Ag segregation. Extensive experimental research works were carried out for optimizing suitable growth parameters for flat monolayer deposition of Cr on Ag(001). The optimum growth temperature was ascertained to 428 K yielding maximum intensity for the c(2x2) half-order spots in Low Energy Electron Diffraction (LEED). Other parameters such as deposition rate, annealing temperature and substrate surface quality are crucial for a highly ordered phase. Our experimental results are consistent with the presence of a p(1x1) Ag overlayer on top of the Cr monolayer, suggesting a Ag/Cr/Ag(001) sandwich structure⁴, which was supported by our DFT calculations. Since the Cr monolayer is buried under the monolayer of Ag, the observed fractional-ordered LEED spot intensity is almost half compared to the theoretically predicted value. The core level electronic structure of the AFM Cr monolayer was investigated by Xray Photoemission Spectroscopy analysis. The valence band dispersions along the high symmetry directions were probed by Angle Resolved Photoemission Spectroscopy studies.

Synergistic Interplay of Defect Density and Temperature: A Comprehensive SCAPS-1D Numerical Investigation in CdTe Solar Cells

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Abstract. In this paper CdS/CdTe heterojunction solar cell is stimulated using SCAPS-1D software streamlining the architecture by excluding hole transport layer. Device optimization is investigated with variation of acceptor carrier concentration and mobilities (hole and electron) of absorber layer and donor carrier concentration and mobilities (hole and electron) of buffer layer. Thus, this meticulous optimized structure produces high output values of Voc=1.01 V, Jsc=28.97 mA/cm², F.F.=85.78% and efficiency=25.17%. The performance of the optimized solar cell is also scrutinized across diverse factors including acceptor and donor defect densities and working temperature. Comparative analysis of the present work with prior reported studies underscores its uniqueness. Consequently, this device configuration can be fabricated experimentally to enable further advancements in solar cell technology.

H1-0006

Studies of Sn Thin Films Growth on Metal Substrates

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Abstract. Metallic tin (Sn) was grown on three metallic substrates Ag(111), Ag(001) and W(110) both at room temperature (RT) and high temperature (HT) (473 K for Ag and 673 K for W). The surface structure of the grown films was studied using low energy electron diffraction (LEED). $(\sqrt{3} \times \sqrt{3})R30^{\circ}$ LEED pattern was observed for Sn growth on Ag(111) not only for 1/3 monolayer (ML) but also for the highest coverage studied for both grown temperatures with only more sharp LEED spots appeared at HT. 1 ML Sn was equally distributed in three substrate Ag layer where each Sn atoms replace every third Ag atoms forming bulk Sn-Ag layer having same surface structure. Sn on Ag(001) formed mainly $p(2\times2)$ and $c(2\times2)$ LEEDfor submonolayer coverage for both RT and HT growth and finally formed a pseudomorphic layer for 1 ML coverage evident from $p(1\times1)$ type pattern. For higher coverage it also formed bulk alloy but with a segregated Ag layer on top confirmed by $p(1\times1)$ along with a $c(2\times2)$ LEED pattern. Only in the case of Sn growth on W(110) no alloy formation was noticed for either submonolayer or few ML coverage at both temperatures. Mainly a stable (1×4) type surface structure was formed by overlayer Sn for higher coverage as it occupied the different energetically available positions on the W(110) surface.

Investigation of Optical Properties of Dielectric Tantalum Pentoxide for Thermal Management

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Abstract. Tantalum pentoxide is one such substance that has been regularly utilized for numerous applications as an antireflective layer, including batteries and MOF-based capacitors. Due to its affordability at a lower cost compared to other dielectric materials like Hafnium Oxide having similar optical, electrical, and morphological properties, our attempt is to apply it for a different purpose, i.e., a spacer layer sandwiched between two metals to fulfill the demand of thermal management using thin film heterostructures or radiative cooling technology. The fabrication method and optical characteristics of tantalum pentoxide on BK-7 substrate have been explored in this paper. The optical studies having Vis–NIR range indicated high transparency in visible region (average transmission~ 80%). The thickness of the films was measured through the Filmmetrics F10-RT thin film analyzer and the values were compared to set values during deposition. Consequently, a technique to illustrate its use on glass doors, windows and rooftops has been suggested by evaluating the optical constants of such coatings.

H1-0008

Close Space Sublimation Growth of Single-phase CuI Thin Films and Evaluation of Structural and Electronic Properties

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Abstract. Binary metal halide, Copper iodide (CuI) is a versatile p-type transparent conductor that has been shown exceptional functionalities towards optoelectronic and thermoelectric applications. Properties such as transparency and conductivity are very sensitive to the morphology, and Cu and I defects. In this study, we report success in preparation of CuI thin films through cost effective close space flux sublimation of CuI powders in vapor transport tube furnace under the optimized pressure (20 mBar with Ar flow) and temperature (400 0 C) conditions. As-deposited samples are found to show single phase CuI with I deficiency, however, post iodization led to improve crystallinity and reduce I vacancies, as revealed from X-ray diffraction and Raman analysis. The bandgap of the thin film is about 2.9 eV and four-point electrical measurements found to show conducting behavior establishing the continuity of thin films. The success in CuI thin film preparation through close space sublimation could pave a way to prepare large area films at low cost.

Electron Beam Deposition of Thin Titanium Films and Its Thermal Oxidation to Form Rutile TiO₂ Thin Films

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Abstract. Titanium is a very useful biocompatible metal which is widely used in the biomedical fields for manufacturing bone anchoring devices as well as cardiac valves and accessories. Compared to other implanting metals, Ti is found advantages for its higher strength and fatigue-resistance as well as its excellent resistance against corrosions. The absorption mechanism of proteins and interaction pathway of host tissue with the Ti surface is very crucial for any clinical applications. However, to examine the protein interaction successfully, a smooth surface morphology of Ti is required to biomimicry the model system. In addition, Ti film surface morphology can significantly influence its surface oxidation process. Apart from Ti films, titanium dioxide (TiO2), based nanostructures are extensively used in sensors, solar cell, and energy storage devices. Hence a detailed understanding of the Ti film formation and its controlled oxidation process are of high scientific as well as technological interest.

Within this work, we will study about the formation of thin Ti film and its thermal oxidation process. High purity Ti was deposited on the quartz substrates using an electron beam evaporation technique, conducted under a high vacuum condition keeping the base pressure below ~10⁻⁵ mbar (HindHighVac). In order to form oxide layers, controlled thermal oxidation of the as-deposited Ti films has been performed in air ambient condition, using a muffle furnace (TEMPCON). Thermal oxidation was conducted at various temperatures for different duration. Structural, morphological, chemical, optical and electrical properties of these oxide layers have been investigated using various surface characterization techniques such as x-ray diffraction (XRD), scanning electron microscopy (SEM), Raman spectroscopy, and x-ray photoemission spectroscopy (XPS). Formation of rutile TiO2 phase is confirmed from XRD and Raman spectroscopy whereas SEM imaging suggests a smooth and homogeneous growth of Ti and oxide layers, appear with a nanometer scale granular surface morphology. All finding are explain in terms of surface thermodynamics and chemical reactivity.

H1-0010

Growth and Characterization of Ag₂ZnSnSe₄ Thin Films

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Abstract. Ag₂ZnSnSe₄ (AZTSe) thin films were synthesized using a two-step procedure that involved selenization at 400 °C in a tubular furnace while varying the argon pressure from 10 mbar to 500 mbar. The precursors (Sn/Se/ZnSe/Se/Ag/Se) were sequentially evaporated under high vacuum in 4-fold stacks. The elemental depth profile (SIMS) showed a uniform distribution of constituent elements. The X-ray diffraction studies revealed similar diffraction pattern with a preferred orientation along (112) plane, indicating the formation of kesterite-type AZTSe for all the selenization pressures. Appreciable changes in morphology have been noticed with increase in selenization pressure from low dense irregular morphology to compact pebbles morphology. All the samples showed high absorption coefficient (>10⁴ cm⁻¹). Nominal variation in the band gap from 1.32 to 1.36 eV was found with an increase in selenization pressure. The Hall Effect measurements reveal that all the films are *n*-type conductive. The precursor stack film selenized at 100 mbar exhibit a high mobility of 7.94 cm²(Vs)⁻¹ and resistivity of $2.61 \times 10^4 \,\Omega$ cm.

Temperature dependent growth study of isoindigo-BTBT for fabrication of transistor

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Organic semiconductor thin films are one of the key components in organic electronics. Their structure, crystallinity, and morphology can significantly influence the properties and performance of the devices. The thin film growth behaviour of organic semiconductors can be affected by the molecular shape, substituents, growth conditions, and so on. Thus, understanding the growth mechanism and controlling the growth process is challenging especially for spin coated film, but it is crucially important. In this work, we have studied the morphological and structural growth of Isoindigo-[1]benzothieno[3,2b]- benzothiophene (Isoindigo-BTBT) polymer thin films grown on SiO2/Si (100) surfaces as a function of the annealing temperature using atomic force microscopy (AFM), X-ray diffraction (XRD), X-ray reflection (XRR) measurements. From the fitted XRR curves using Parratt's recursion method, a schematic representation of the internal structure of the polymer film at different temperatures is modelled. It is also observed how the quality of crystallinity, defined atomic layers, interconnection between domains, density of material and relatively lower roughness of the organic semiconducting material helps to improve mobility of OFET. It offers better understanding of the influence of spin coating speed and annealing temperature on the thin film growth behaviour, providing guidance for future developing high-performance organic field effect transistors (OFET).

H1-0012

Combine Influence of Surface Roughness and Deformation on the Performance of Elastohydrodynamic Lubrication

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Abstract: This article aims to investigate theoretically the performance of a transversely rough Electrohydrodynamics lubrication by considering bearing deformation. The Stochastic modeling of Christensen and Tonder has been adopted for calculating the effect of transverse surface roughness. The pressure distribution is obtained by deciphering the associated stochastically average Reynolds equation. All results, customized in a graphical way established that the transverse roughness in conjunction with the deformation has a robust adverse effect on the performance of the bearing system. This article may also have triumphed some measures for extending the life span of the bearing system,

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Effect Of Annealing On Chemical Bath Deposited Copper Sulfide Thin Films

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Abstract. Copper sulfide (CuS) thin films are a promising material for optoelectronic devices, including solar cells, touch screens, and light-emitting diodes (LEDs). They have the potential to be used as a ptype transparent conducting material (TPCM), which is a material that is both transparent and conductive. In this work, CuS thin films were deposited using chemical bath deposition (CBD) and then annealed to study the effects on their structural, compositional, optical, and electrical properties. X-ray diffraction (XRD), scanning electron microscopy with energy dispersive spectroscopy (SEM-EDS), ultraviolet-visible (UV-Vis) spectroscopy, and Hall effect measurements were used to characterize the annealed films. Calculation of Figure of Merit values helped to find the best samples.

H1-0014

Temperature Dependence of TiO₂ Thin Films by Spray Pyrolysis Technique

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Abstract. Titanium dioxide (TiO₂) thin films were prepared onto glass substrates at a substrate temperature of about 400°C, 450°C and 500°C by Spray Pyrolysis technique. The prepared thin films were characterized by X-ray diffraction, Scanning electron microscope and also subjected to UV-Vis studies in order to characterize the structural property, surface morphology and optical properties. The diffraction peaks from XRD were indicates that the structural property (Anatase phase) for TiO₂ thin films. The results showed that at doping the intensity of (101) plane decreased which may be due to mobility of Titanium and Oxygen atoms which leads to reduction in the nucleation of crystallization phase of anatase TiO₂. The SEM structure revealed a uniform and evenly distributed grains across the substrate surface. Bandgap calculated from UV-Vis spectra.

Large scale surface cratering on Al thin film using low energy ions

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Abstract. Ion beam-induced modification of Al thin films of thickness 25 nm and 50 nm was investigated. Irradiating the films by 100 keV Ar $^+$ ions with varying ion fluence leads to the changes in the morphology and composition, which were analysed using Field Effect Scanning Electron Microscopy (FESEM), Atomic Force Microscopy (AFM), Rutherford Backscattering (RBS) Spectrometry. SEM and AFM images shows the presence of large, uniformly shaped circular craters with distinct rims. These craters exhibited varying diameters, ranging from 200 nm to 1 μ m for the 25 nm films and 100 nm to 2.5 μ m for the 50 nm films. The presence of a pronounced dependence on fluence is apparent, as both the density (number of craters per unit area) and diameters exhibit variations with changes in ion fluence, transitioning from the regime of single ion impacts to that of multiple ion impacts. The RBS spectra do not exhibit any discernible evidence of ion beam induced mixing. However, the sputtering of films is clearly observable, as anticipated. The integrated peak area of the aluminium peak decreases by 60% and 55% for 25 nm and 50 nm films, respectively, when subjected to the highest fluence employed.

Vibrational Spectroscopic, 13C NMR, DFT Studies on Chlorofullerene (C₆₀Cl₆): A Potential Bioactive Agent

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Abstract. The present work comprises the systematic quantum chemical studies on Chlorofullerene (C₆₀Cl₆). The molecular structure of C₆₀Cl₆ was optimized by DFT/B3LYP method with 6-31G(d,p) basis set using Gaussian 09 program. The infrared and Raman spectra were simulated and assigned for C₆₀Cl₆ molecule. Carbon – chlorine stretching vibrations are found to be in the range 150-900 cm⁻¹ and the chains are strongly affected with the radial vibrations of the carbon sphere. Ground-state optimized geometries of the molecules are calculated without any geometrical restriction, except those enforced by symmetry. The molecules are found to be minima on their respective potential energy surfaces as revealed by the lack of imaginary frequencies. The optimized structures have been subjected to Gauge including atomic orbital (GIAO), the chemical shielding tensors using B3LYP/6-31G(d,p) in solvent phase in order to calculate 13C chemical shift values with respect to trimethylsilane (TMS) as computational reference. Molecular reactivity and stability were investigated using the Frontier molecular orbitals (FMO) analysis. The molecular electrostatic potential (MEP) mapping provides a valuable information regarding the net electrostatic effect produced by total charge distribution of the molecule. Chlorofullerenes are considered to be promising compounds for the investigation of biological action which show pronounced anti-HIV action and low toxicity. Hence, these results pave the way for designing the biocompatible molecules which will be useful in the field of carbon nano medicine and pharmaceutical applications.

I1-0002

A DFT Study on Phase Transition, Electronic Structure, Optical and Electronic Properties of PbTe

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Abstract. This study is about the FP-LAPW (Full Potential Linearized Augmented Plane Wave) method used for density functional theory (DFT) to study the structural phase transition of PbTe under pressure. Our results indicate that a structural transformation from NaCl to CsCl occurs at 13.9 GPa, which is in good compatibility with search observations. To determine the soil condition properties of the B1 crystalline structure, the total energy was found to be FUNCTION OF THE UNIT CELL VOLUME. The PBA-GGA exchange-correlation potential was utilized to evaluate the density of states, electronic band structure, and optical spectra. Novelty is we theoretically determined the second-order elastic constants, as well as thermo-mechanical properties of PbTe. Our computed results are in line with available theoretical and experimental data.

First principles investigation of structural and electronic properties of tungsten nitrides under pressure

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Abstract: The structural, electronic and mechanical properties of several phases of noble metal nitrides WN are investigated by the ab initio total energy calculations within the frame work of density functional theory. Among the four crystallographic structures that have investigated, the hexagonal WC structure is more stable than the cubic ones. The calculated lattice parameters are in good agreement with the available results. A pressure-induced structural phase transition from WC (Bh) to ZB (B3) phase is observed in WN. The elastic properties of four structures are calculated, which are in consistent with the obtained theoretical and experimental results.

I1-0004

Tetrogonally Distorted Full-Heusler Alloy

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Abstract. Tetragonal Heusler alloys have wide range of application in spintronics due to their high Perpendicular Magnetic Anisotropy (PMA) which is responsible for spin transfer torque (STT) devices. The objective of the research work is to study the tetragonal distortion in the Full-Heusler alloys Co2NbSn and Co2TaSn. The electronic properties of the full-Heusler alloys Co2NbSn and Co2TaSn are studied using pseudopotential method-based Density Functional theory (DFT) using Quantum Espresso. The Generalized Gradient Approximation (GGA)- PBE is used as the exchange correlation potential. The electronic band structure and the Density of States (DOS) of the alloys in cubic L21 phase reveal the characteristic of ferromagnetic metal with high DOS at the Fermi level (EF) which indicates the instability of the alloy. The alloys were subjected to tetragonal distortion and found that there is decrease in Density of Sates (DOS) at the Fermi level due to the splitting of states. These alloys are stable in tetragonal phase than cubic L21 phase. The mechanical properties of the alloys are studied to determine the mechanical stability of the alloys in tetragonal phase. The obtained phonon dispersion curves indicate that these alloys are thermodynamically stable in tetragonal phase.

Carcinogenic dioxane detection using engineered 2D Ge monolayer: An ab-initio study

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Abstract. We have calculated the structural, electronic, and vibrational characteristics of 2D germanium (Ge) monolayers in all of their three different structural configurations planner, buckled and puckered using DFT calculations. Total energy calculations show that the 2D puckered structure has the lowest energy. Among them planer and puckered structures show metallic behavior, which in order of 0 eV while buckled shows direct bandgap of 0.075eV. We have also calculated phonon dispersion curve to understand its mechanical stability, the buckled structure produces positive phonon vibrations (~4 cm⁻¹), indicating that it is the most stable structure.

I1-0006

Understanding of efficient photocatalyst for water splitting using As monolayer: DFT study

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Abstract. We have examined the structural, electronic, and vibrational characteristics of 2D Arsenene (As) monolayers in their three different structural configurations planner, buckled and puckered using density functional theory (DFT) calculations. Total energy calculations as well as phonon dispersion curve reveals that the 2D puckered structure has the lowest energy and also dynamical stable. The 0 eV energy band gap causes the planner structure to exhibit metallic behaviour. The indirect band gaps of the buckled and puckered systems are 1.92 eV and 1.73 eV, respectively. Further, we adsorb the water molecule (H₂O) on the sheet and found that the adsorption energy is -3.42 eV show stability after the adsorption, which has a potential application in photocatalysts.

Adsorption properties of sulfurous gas based on Fe, Co, Ni decorated Sb monolayer: A first principles study

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Abstract. The adsorption properties of H₂S and SO₂ gas on Fe, Co, and Ni decorated antimony monolayers are reported using density functional theory. We have systematically investigated the structural, electronic, and vibrational properties of 2D Sb monolayer two structures: planner and buckled. Negative total energy for the buckled and planar structure indicate structure stability. The band gap for the buckled and planar structure was 1.41 eV and 0 eV, respectively. Band gap indicates semiconductor property for buckled antimony and metallic property for planar antimony. From the partial density of state (PDOS) we analyze that the majority contribution is obtained by the 5p orbital for both structure. Our results shows that buckled monolayer has potential application for the sulfurous gas sensing.

I1-0008

The First-Principles DFT Computation Of Electronic Structures Of Cubic Perovskite SrMnO₃ Sonu Sharma

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Abstract. First principles calculations have been made on cubic perovskite SrMnO₃ to investigate structural, electronic and magnetic properties. The computed lattice parameters and bulk modulus by using PBEsol exchange correlation functional are found to show good agreement with the experimental values and earlier reported theoretical values. The analysis of both density of state (DOS) and band structures shows the half metallic ferromagnetic ground state in the compound, which suggests its potential applications in spintronic devices. Mn-3d and O-2p orbitals near Fermi level are responsible for the ferromagnetic behavior and total magnetic moment of the compound.

Investigation of Electronic Structure and Phonon Frequencies of Quaternary Heusler Compound LiTiCoSn

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Abstract. In this study we investigated the structural and electronic properties and phonon dispersion frequencies of quaternary Heusler LiTiCoSn compound using the first principles calculations. The band structure and density of states has been studied in electronic structure calculation by the employment of generalized gradient approximations. In study we found that the compound is indirect band semiconductor in nature. The non-magnetic behaviour of the presented compound is calculated by the Slater-Pauling rule. Further the phonon dispersion curves are calculated via density functional theory. The calculation reveals that the compound LiTiCoSn is dynamically stable in cubic phase as there are only positive phonon frequencies. Therefore, these theoretical findings may provide strong justifications for the further experimental investigations of the material.

J1-0001

Magnetic Properties of Mn_{1.5}Fe_{1.5}Al Heusler Alloy

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Abstract. Heusler alloys are ternary intermetallic alloys with the general formula: X₂YZ and XYZ. Heusler alloys have governed a lot of attention due to their different functional characteristics and prospective technological uses in spintronic devices, sensors, actuators, and refrigeration. The Manganese-based Heusler alloys are among the most fascinating because of their complex physical properties and ease of availability. The Mn-based Heusler alloys have recently been studied in the context of the topological Hall effect, skyrmions, spin Hall effect, spin transfer torque, etc. One such alloy is Mn_{1.5}Fe_{1.5}Al. A detailed study of magnetic properties of polycrystalline Mn_{1.5}Fe_{1.5}Al Heusler alloy has been done by DC and AC susceptibility, magnetic memory, magnetic relaxation, unidirectional exchange bias and thermoremanent magnetization measurements. The Mn_{1.5}Fe_{1.5}Al alloys crystallize in a β-Mn cubic structure. These alloys exhibit sharp peak at spin glass freezing temperature $T_f \approx 34.5$ K with large negative Curie-Wiess temperature ($\theta_W = \sim 639$ K), which indicates strong antiferromagnetic interaction and large frustration. The temperature and field variation of magnetization indicates the presence of a spin glass nature. The analyses of field dependent of irreversible temperature, exponential dependence of coercivity and remanence, frequency-dependent shift of T_f in AC susceptibility measurements which follows the Vogel-Fulcher law and critical slowing down approach, shifting of MH hysteresis loop in field cooled mode, magnetic memory, and relaxation effect below T_f and asymmetric behavior in magnetic relaxation confirms canonical spin glass nature in the studied alloy.

J1-0002

Structural and Magnetic Properties of Mixed Valence Manganite Perovskites

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Abstract. Samples are prepared using a solid-state reaction method. Rietveld refinement of room temperature X-ray diffraction study reveals that the samples are single phase and crystallize in rhombohedral crystal (R-3c) structure. Magnetic data suggest the ferromagnetic (FM) to paramagnetic (PM) transition at Curie temperature (T_C). The antiferromagnetic correlations dominantly take place at low temperatures. Magnetization versus magnetic field (M-H) data fitting suggests a structural defect and susceptibility increase by order one.

Investigation of structural and magnetic properties of ball milled and post annealed Ni₅₀Mn₃₆Fe₂Sb₁₂ Heusler alloy

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Abstract. Heulser alloys are promising materials due to its tunable magnetic and related properties that may provide outstanding functionality. In present work we demonstrate the preparation and investigation of Ni₅₀Mn₃₆Fe₂Sb₁₂ ball milled Heusler alloy. Furthermore, we report the effect of ball milling and its annealing effect on the structural, magnetic and exchange bias properties of Ni₅₀Mn₃₆Fe₂Sb₁₂ Heusler alloys. The ball milled samples exhibit coexisting austenite and martensite phases at room temperature, while annealing suppresses the austenite phase completely. Ball milling was found to reduce the particle size, which resulted in the weakening of the ferromagnetic properties. An exchange bias field of 111 Oe and coercivity of 826 Oe were observed at 5 K in the as-milled sample. Annealing causes an increase in the ferromagnetic ordering and a decrease in the interfacial exchange coupling, resulting in a decrease of both exchange bias and coercivity in the annealed samples. The combination of cost efficient synthesis technique and tunable magnetic properties opens a new path to the possible of mass production of Heusler alloys for various applications.

J1-0004

Quantum Dimer Model With Exact Columnar Ground State

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Abstract. An antiferromagnetic spin- $\frac{1}{2}$ model is considered on a square lattice having exchange interaction up to third nearest neighbors. The model is constructed in such a way that it shows an exact dimer ground state for a particular ratio of exchange interactions ($J_1:J_2:J_3=6:2:1$). The ground state energy and spin-spin correlations of the model, obtained through Lanczos diagonalization, reveal a finite spin gap. These results align with the exact analytical findings achieved using projection operators. In the framework of triplon mean-field theory, the model shows a Bose condensation of singlets, forming a magnetically disordered columnar dimer ground state at the exactly solvable point. As we vary the interactions from this exact point, triplets disperse within a background of singlets, revealing a diverse range of complex many-body phases.

Effect of Nonmagnetic Zn on Pinning Properties of Bulk YBCO Superconductor

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Abstract. Replacing Cu by nonmagnetic Zn in YBCO affects current-voltage (*IV*) characteristics strongly. A strong reduction of ~ 43.5 K in critical temperature, T_c , and nonlinear behavior of *IV* have been observed. Dependence of the transport critical current density, J_c , as a function of temperature, T_c , reveals a change in the vortex pinning mechanism. However, an exponent related to the nature of pinning remains almost unchanged over a range of temperature. We have attributed the reduction in T_c and J_c by nonmagnetic Zn to the suppression of the number density of the Cooper pairs.

J1-0007

Effect of Spin Disorder on Magnetization and Susceptibility Resulting from NdNi₈ Sub-lattice in Nickelates

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Abstract. Impact of arrangement of spins of NdNi₈ sub-lattice in the nickelate (NdNiO₂) system have been studied by altering the distance (r_{ij}) between neighboring spins. We have calculated both magnetization (M) and susceptibility (χ) as a function of r_{ij} at a combination of a constant temperature (T) and magnetic field (H) for a specific finite perturbation limit (Δ) . Inter-spin separation, r_{ij} has almost no effect on M for the non-perturbation limit, $\Delta = 0.0$. A curvature in M have been observed for the increase of r_{ij} at $\Delta = 0.3$. Variation of M and χ with r_{ij} is prominent around low H and low T.

Unusual high pinning exponent in Ni doped YBCO superconductor

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Abstract. We have studied current-voltage (IV) characteristics of (i) the pure YBCO and (ii) the Ni doped YBCO at several temperatures (T) below respective critical temperatures, T_c . IV characteristics have been used to extract total critical current density (J_c) and granular critical current density (J_cG). Following a power law equation, $J_c(T)$ is analyzed and an exponent is extracted. The role of the magnetic Ni²⁺ replacing Cu(2) of superconducting CuO₂ planes on the pinning exponent is found to be very significant.

J1-0009

Effectiveness of Sn Nanoparticles as Pinning Centres in YBCO Superconductors

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Abstract. We have explored how nanoparticles of Sn and SnO₂ impact on the vortex pinning mechanisms in granular YBCO superconductors. Low densities of Sn and SnO₂ have been added into the inter-granular network of YBCO. The current – voltage (IV) characteristics have been used to study the temperature (T) - dependent exponent (η) within the framework of the Berezinskii – Kosterlitz – Thouless (BKT) phase transition. Applying the Ambegaokar – Halperin – Nelson – Siggia (AHNS) theory, we have determined the superfluid phase stiffness (J_s) as a function of T. Additionally, T-dependent transport critical current density (J_c) has been analyzed to understand the differences in pinning mechanisms.

Large Magnetocaloric Behavior of Ceramic GdFe_{0.7}Al_{0.3}O₃ Compound

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Abstract. Aluminum doped ceramic orthoferrite GdFe_{0.7}Al_{0.3}O₃ (GFAO) compound was chemically synthesized following solid-state-reaction mechanism. XRD intensity-profile analysis categorized the GFAO material as orthorhombic crystal group possessing *pbnm* symmetry through Rietveld refinement technique. The ZFC and FC thermomagnetic curves coincide throughout in the temperature range of 2.7 K to 300 K. Analysis shows the paramagnetic nature of GFAO compounds while the coincidence of FC-ZFC curves reflects the absence of thermal hysteresis in the sample. Modification of spin structure is observed at Fe³⁺ site due to the doping of Al³⁺ which is well observed in M-H hysteresis loop at low temperature (2K). The M-H loop further indicates magnetic hysteresis is negligible. For a magnetic field change of 5T, the peak value of magnetic entropy change of GFAO compound reaches the value 17.15 JKg⁻¹K⁻¹ in low temperature region, and it establishes the GFAO ceramic compound as a potential candidate for low temperature solid-state refrigeration.

J1-0011

Anharmonic Phonon-Electron Problem of Iron Base High Temperature Superconductors A.P. Singh¹, Yogendra Kumar²

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Abstract. The problem is handled using double time thermodynamic Green's function theory because the consequences of anharmonicity on the phonon-electron problem of high temperature superconductors are virtually unexplored. This theory consists of the Hamiltonian that includes inputs from the harmonic, anharmonic phonon fields, and localized phonons phonon fields, as well as electron—phonon interactions. This technique can forecast the generation and decay of Cooper pairs in superconducting crystals automatically. In the general paradigm, expressions for electron density of states(EDOS) and phonon density of states (PDOS) are established, which are able to depict a vast variety of dynamical features of high temperature superconductivity.

The temperature dependence of PDOS and EDOS has been found as a unique feature of the theory, which certainly becomes the outcome of the anharmonic interactions. The presence of electron—phonon interaction parameters in each term is an additional and new feature of the theory.

$Coherence\ Length\ and\ Transport\ Critical\ Current\ Density\ in\ Y_3Ba_5Cu_8O_{18-\delta}/Co\ Composite\ Superconductor$

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Abstract. We have investigated how the low concentrations of ferromagnetic Co-nanoparticles in intergranular networks of multilayered Y₃Ba₅Cu₃O_{18- δ} (Y358) superconductor affect the coherence length (ξ_c) at absolute zero temperature and critical current density, J_c . Fluctuation induced conductivity (FIC) is used to extract ξ_c (0). An increasing trend of ξ_c (0) with increasing concentration of Co is observed attributed to the deterioration of the superconducting properties. We have extracted J_c from current-voltage (*IV*) characteristics in the phase transition region. Reduction in J_c has also been observed with increasing the concentration of Co-nanoparticles.

J1-0013

Review on Electrode Materials for Super Capacitor Energy Storage

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Abstract. Super capacitors have gained increasing attention as an energy storage technology due to their high power density, fast charging and discharging rates, and long cycle life. One of the key factors that affect the performance of super capacitors is the electrode material. Various types of electrode materials have been developed and investigated, including carbon-based materials, metal-based materials, conductive polymers, and emerging materials such as MXenes and metal-organic frameworks. Each type of electrode material has its own unique characteristics and advantages, which can affect the performance of the super capacitor in terms of energy density, power density, cycle life, and cost. In this review paper, we provide an overview of the characteristics and performance metrics of super capacitor electrodes and discuss the advantages and disadvantages of different types of electrode materials. Additionally, we highlight emerging electrode materials that have shown promise for improving the performance of super capacitors and discuss the potential future directions for research in this field.

Studying the Structural, Magnetic and Dielectric properties of cobalt substituted R type Hexaferrites

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Abstract. A new type of Co^{2+} substituted R type hexagonal ferrite $Sr_{1-x}Al_2Co_xFe_4O_{11}$ (x=0.0,0.1,0.2,0.3 and 0.4 was synthesized by simple heat treatment method. The obtained precursors were heated at 950 °C for 3 h and then characterized using various instrumental techniques like X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR) and Vibrating sample magnetometer (VSM). The XRD pattern of all the samples depicts R phase with an additional Fe_3O_4 phase. The magnetic properties i.e., Saturation magnetization (Ms), Coercive field (Hc), and Remanent magnetization (Mr), were estimated from the ferromagnetic hysteresis behaviour of the samples measured using Vibrating Sample Magnetometer (VSM). The non linear variation in magnetic parameters was observed with the increase in doping content.

J1-0015

Magnetic octupole domains in the non-collinear antiferromagnetic Weyl semimetal Mn₃Ge

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Abstract. Geometrically frustrated magnetism and topology in electronic systems, individually, have been at the forefront in quest for quantum phases for futuristic quantum applications. A new class of room temperature antiferromagnets, Mn₃X (X = Sn, Ge) hosts two features. The topological nature (Weyl points) of their magnetic structure gives rise to a spontaneous Hall effect whose sign can be switched extremely rapidly at terahertz frequencies. This results from the reversal of magnetic octupole domains rather than a conventional magnetic dipole picture. Such states are of potential interest for applications in ultrafast non-volatile data storage and information processing technology at room temperature. In this work, we studied the magnetic properties of Mn₃Ge by magnetic atomistic simulations. We confirmed the magnetic exchange (symmetric as well as asymmetric (Dzyaloshinskii-Moriya) interaction parameters) by matching the obtained magnetic phase transition to the reported experimental value. Building on this, we demonstrated the inverse triangular structure with magnetic octupoles as the ground state of the system. We firstly obtained the magnetic octupole domain walls in Mn₃Ge and investigated its behavior as a function of temperature and applied magnetic field. This offers a better understanding of the fundamental physics of strongly interacting electrons and spins in topological materials.

Magnetic Studies of Ni (Mg, Co) Fe₂O₄ Using Auto-Combustion Method

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Abstract. This article presents the magnetic studies of divalent metal ions substituted nickel ferrite. Divalent metal ions such as Mg⁺² and Co⁺² were substituted in pure Nickel ferrite (NiFe₂O₄) with the basic composition Ni_{0.5}M_{0.5}Fe₂O₄ (here, M= Mg⁺², Co⁺²), which were synthesized by auto-combustion method using, nitrate-citrate method. Synthesized samples were sintered at 950°C and investigated for various properties. Phase of the synthesized samples were probed by X-ray diffraction (XRD) studies. Peaks observed in the XRD spectrum confirms the single phase spinel cubic structure for the divalent metal ions substituted NiFe₂O₄. Using FESEM, surface morphology of the samples has been investigated. For the proposed nano-powder samples magnetic measurements were done at RT using Vibrating Sample Magnetometer (VSM).

J1-0017

Mn-Ni-Co-Sn full Heusler Alloy: Investigation of Structural, Magnetic and Exchange Bias Properties

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Abstract. In the present report, we have studied the structural, magnetic, and exchange bias properties of a Mn rich Mn-Ni-Co-Sn full Heusler alloy. Present alloy exhibits the tetragonal structure at room temperature, and is found to undergo a first order structural (i.e. martensitic) transition at around 335 K. The low temperature frustrated magnetic state of the martensite phase for this alloy has been investigated by means of the DC magnetization and frequency dependent AC susceptibility measurements, which confirm the coexistence of spin glass (SG)/ferromagnetic (FM) phases at low temperatures. A large exchange bias field of 990 Oe has been observed at 2 K after field cooling the alloy at 10 kOe, which is comparable with the other literature reports. This is attributed to the large exchange anisotropy present at the SG/FM interfaces. The cooling field strength effect on the exchange bias properties has also been studied here.

Nature of the magnetic transition in multicomponent intermetallic compound Dy0.33Ho0.33Er0.33Al2

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Abstract. Rare earth Laves phase intermetallic compounds RAl2 (R = rare earth) have been extensively studied for their magnetic and magnetocaloric properties. These compounds order ferromagnetically (TC) at low temperatures and TC scales with de Gennes factor. A polycrystalline multicomponent Laves phase intermetallic compound Dy0.33Ho0.33Er0.33Al2 has been synthesized by arc melting and characterized using powder X-ray diffraction and magnetization experiments. The sample crystallizes in a cubic structure (space group Fd3m) at room temperature. Upon cooling, the compound Dy0.33Ho0.33Er0.33Al2 undergoes paramagnetic to ferromagnetic transition around 33 K followed by a spin reorientation transition around 7 K [1]. The order of magnetic transition plays a vital role in determining the overall performance of a magnetic refrigerant. This work is focussed on determining the nature of transition by analysing the magnetic data using different methods such as Arrott plots, universal curve fit and the Inoue-Shimizu model. Magnetocaloric properties have also been studied using the magnetization and heat capacity data.

J1-0019

Impact of Thermal Noise in Magneto Resistance Tilted Polarizer based Spintronic Oscillator - A Macro-spin Insight

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Abstract. In the present work, we have modeled a heterogeneous Magneto Resistance Tilted Polarizer based Spin Torque Nano Oscillator [MRTP-STNO] theoretically. The precession of magnetization dynamics led by Spin Transfer Torque [STT] is studied numerically by solving the equation called Landau-Lifshitz-Gilbert-Slonczewski [LLGS]. Here, β is the independent tilt angle of fixed layer and θ is the angle between free layer magnetization and the easy axis of the device respectively. Both the angles can be varied from 10° to 90° as an increment of 10° . The maximum frequency of the modeled device is of about 235.5 GHz and PSD of $1.74~\mu\text{W/mA}^2/\text{GHz}$ in the absence of thermal noise and in the presence of thermal noise the frequency as well as the corresponding PSD is recorded as 215.4~GHz and PSD of $1.70~\mu\text{W/mA}^2/\text{GHz}$. The author insinuates that the modeled device is applicable towards the High-Frequency applications and opens a new platform for forthcoming spin-based devices during its practical usage.

Structurally Driven Magnetic Influences in Sputtered Nano Ni Films

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Abstract. In order to investigate structurally driven magnetic influences in sputtered nano Ni films, two sets of Ni films with varying thicknesses have been deposited on a Si (111) oriented substrate. These nanofilms have been produced employing a RF-sputtering system at room temperature. AFM images illustrate that these nanoscale thin films have been formed very smoothly over the Si substrate. A strong texture along Ni (111) plane is observed through GIXRD characterization. The quality of the nano Ni films is demonstrated by the effectively resolved Kiessig fringes in the XRR data. The film thickness obtained from linear regression and Fast Fourier Transform (FFT) analysis of the XRR data is in good consistency with the as-prepared nominal thickness. The ferromagnetic resonance (FMR) data reveals that, due to differences in surface anisotropy and interface roughness, the resonance field (H_R), line width (Δ H), and effective magnetization (M_{eff}) are lower in the thin film compared to the thick one. In the thicker Ni film, multiple resonance peaks are observed. The thicker Ni film exhibits characteristics of being more soft ferromagnetic compared to the thin one. Easy axis of magnetization is found to be along the film surface.

J1-0021

Electrical and Magnetic properties of Ba_{0.7}Sr_{0.3}TiO₃ - Co_{0.65}Zn_{0.35}Fe₂O₄ Composite Multiferroics
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Abstract. Ferromagnetic $Co_{0.65}Zn_{0.35}F_{e2}O_4$ (CZFO) nanoparticles were embedded in a bulk ferroelectric $Ba_{0.7}Sr_{0.3}TiO_3$ a two-phase magnetoelectrically coupled to form composite system. In this present study the particulate composite system $(1-\Phi)$ $Ba_{0.7}Sr_{0.3}TiO_3$ (BSTO)- Φ $Co_{0.65}Zn_{0.35}Fe_2O_4$ (CZFO) (Φ = 0.1, 0.2, and 0.3) were synthesized using a hybrid synthetic technique (conventional solid state reaction and auto-combustion method). The XRD patterns confirm the formation of tetragonal structure for BSTO and cubic structure for CZFO. The Rietveld refinement technique was performed to extract the atomic level parameters on mixed phase composites. It is noticed that, crystalline size and lattice parameters were reduced with increasing the CZFO content. The M–H loop measurement at room temperature suggests the ferromagnetic ordering for all the composites. Indirect evidence of ME coupling noticed by increasing BSTO content in CZFO, saturation magnetization decreased. The dielectric constant and dielectric loss plot exhibits the Maxwell-Wagner type of polarization with respect to their applied frequency.

Synthesis of PbTaSe₂ single crystal superconductor using CVT method

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Abstract. In the present work, I have reported the successful growth of PbTaSe₂ single crystals by chemical vapour transfer method using single zone tubular furnace. Tiny crystals of 1x1mm² size are obtained whose composition and morphology has been confirmed using XRD, TEM and FESEM.

K1-0001

First Principle Study of Effects of Pressure Variation on the Structural and Mechanical Properties of ZrSiO₃ Perovskite

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Abstract. Mechanical pressure affects the properties of ZrSiO₃ in geological science, materials science and engineering providing valuable information for a variety of applications. In this study, the structural and elastic properties of ZrSiO₃ perovskite were examined using density functional theory. Some of the related physical quantities, such as the bulk, shear, Young's moduli, Poisson's ratio, anisotropic factor, acoustic velocity, minimum thermal conductivity, and Debye temperature were calculated using the Quantum Espresso code. The pressure-dependent elastic constants were studied, it was observed that the elastic constants of the ZrSiO₃ perovskite slightly increase with the rise in pressure. Also, the findings show that ZrSiO₃ can still maintain its mechanical stability and ductility at high pressures up to 100 GPa. The thermal behavior was evaluated by calculating the Debye temperature using the analysis of average sound velocity.

K1-0002

Effect of Dust on Production of Entropy Behind Exponential Strong Shock in Self-gravitating Gas

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Abstract. In this paper, the effect of dust present in the gaseous medium on the phenomenon of production of entropy due to the motion of strong spherical converging shock waves. Assuming the exponentially varying initial density distribution the CCW method has been used to solve the problem for freely propagation as well as under the influence of waves traveling behind the shock front. The dust particles are seeded in the pure ideal gas. The dust particles are inert in nature, solid and spherical in size. They are uniformly distributed in the medium. Maintaining the equilibrium flow conditions, the analytical expressions for the entropy production and change in temperature just behind the shock front under the self-gravitating medium are obtained. The effect of mass concentration of solid particles in the mixture, the ratio of solid particles to the initial density of gas, and the density parameter have been computed numerically and discussed through figures. It is observed that in presence of solid dust particles in the gaseous medium has a significant role in the increase in entropy and temperature for both cases. The inclusion of overtaking waves behind the front in the study also indicates that both the parameters entropy and temperature are further increased. A comparison of results obtained in the case of dust-free gases, and also neglecting the effect of overtaking waves, has been discussed through graphs.

K1-0003

Lattice Dynamical Investigation of Raman and IR Wave Numbers at the Zone Center of Orthorhombic Perovskite LuFeO₃

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Abstract. Herein, we have investigated the Raman and infrared wave numbers of LuFeO₃ orthorhombic perovskite using a short-range valence band force-field model. In our calculation, we employed 9 stretching and 7 bending force constants in the Wilson GF matrix method. Our calculated wave numbers agreed well with the observed wave numbers. The Raman wave numbers were assigned to their specific mode of vibrations. The infrared wave numbers have been calculated and assigned. The potential energy distribution has also been determined to signify the contribution of the force constants toward the Raman and infrared wave numbers.

K1-004

On The Electrical Properties And Temperature-dependent Properties, viz., Viscosity And Relative Density Of Water-based Spinel Zinc Ferrite Ferro Fluids

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Abstract. While studying thermo-acoustic properties of binary, ternary liquid mixtures or that of ferrofluids, one not only need to measure the variation of acoustic parameters like acoustic impedance, hydration number, Rao's constant, Wada's constant, apparent molar volume, apparent molar isentropic compressibility at different temperature values but also need to see whether parameters like relative density, viscosity of the substance changes with change in temperature. This study is of utmost importance because while estimating the acoustic parameters sometimes relative density, sometimes viscosity and sometimes both of it appears in the formula. Electrical properties of the substances are also of similar importance. Hence, investigation of variation of viscosity, relative density of specific ferro-fluids, with temperature is an important area of study. In this communication we have reported variation of viscosity, relative density of water based Zinc Spinel ferrite with temperature. The electrical properties of the water based Zinc Spinel ferrite are also reported. The study is carried out in the concentration range 0.001 M to 0.01 M. At concentration lower than 0.001 M, the behaviour of ferrofluids begins to deviate from the bulk fluid properties and as the concentration approaches 0.01 M, potential aggregation effects and saturation phenomena made the solution not to disperse as desired. The Zinc spinel ferrite is synthesized by sol-gel technique.

K1-0005

Investigation on the Structural and Mechanical Properties of Al/Mg Joints through Friction Stir Welding

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Abstract. Friction Stir Welding (FSW) has emerged as a transformative solid-state joining technique, particularly relevant for creating robust and defect-free joints between dissimilar materials. This study comprehensively investigates the structural and mechanical properties of Al/Mg joints produced through the FSW process with the primary objective of discerning and characterizing the resulting joint attributes and mechanical behaviour, substantiated by quantitative data. Experimental trials encompass an array of FSW processes, incorporating varied rotational speeds within the range of 800 to 1200 rpm, traverse speeds ranging from 30 to 60 mm/min, and tool configurations featuring pin diameters of 4 and 6 mm. Subsequent microscopic evaluations, facilitated by optical and electron microscopy, unveil distinct intermetallic compounds, notably Al3Mg2 and Al12Mg17, within the microstructure of the welded joints. Mechanical analyses comprise tensile testing, with particular attention to the impact of induction preheating. Comparative examination of tensile strengths between preheated and nonpreheated joints demonstrates a significant enhancement of 12.04%, with preheated joints registering a tensile strength of 86.95 MPa as opposed to 77.60 MPa for non-preheated joints. Complementary microhardness testing serves to reinforce the salient effect of preheating on the mechanical attributes of the joints. The findings underscore the pivotal role played by intermetallic compounds in influencing structural integrity and mechanical potency within Al/Mg joints established via FSW. Furthermore, by establishing correlations between process variables and resulting mechanical properties, this study provides essential insights, enabling optimization of the FSW process and advancing our understanding of material response in dissimilar material joining techniques.

K1_0006

Mechanical Properties of AlZr3 Alloy and BMG using Molecular Dynamics Simulations

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Abstract. One of most exciting as well as demanding problems among the researchers associated to the creation of a new generation of exceptionally well-functioning structural alloys in the past few decades has been the syn-thesis of bulk metallic glasses (BMGs). The interesting thing about the BMGs are that they show mechanical strength as well as yield strain comparable to that of crystalline materials. BMGs are new structural materials with a high demand due to their remarkable strength, despite the fact that they have major issues with ductility and lack of work-hardening. However, fundamental knowledge on the composition dependency and mechani- cal characteristics of the metallic glasses are limited till date. Generally speaking, the science of liquids and glasses is significantly less developed than that of crystalline solids. Indeed, we can say one of the biggest problems with the field of research in condensed matter is to comprehend the nature of glass and the transition of glass. In recent years, research into bulk BMGs has rapidly developed and has been extensively investigated in a wide range of applications due to the interesting and unique mechanical properties that are not found in crystalline alloys. The BMGs based on zirconium have drawn attention in terms of both research and application because of their high glass forming ability (GFA) and unique structural characteristics. To understand the mechanical properties of BMGs, it is important to understand their deformation mechanism under different loading conditions. Molecular dynamics (MD) simulation is a very handy tool which can be used to simulate the BMGs in order to study the above mentioned properties efficiently. In this work, MD simulations have been carried out to study the effect of strain rate on various mechanical properties of the AlZr3 bulk alloy under uniaxial tensile

stress. BMG of AlZr3 is also created and its mechanical properties at a constant strain rate is estimated. For this purpose, the semi-empirical potential based on the second nearest neighbor modified embedded atom method (2nn-MEAM) are applied.

K1-0007

Structural Anomaly in Ni Based Transition Metallic Alloys

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Abstract. Polycrystalline transition metallic alloys have been prepared using arc melting method by choosing stoichiometric amount of Nickel (Ni) and Iron (Fe) and were investigated structurally using X-ray Diffraction Technique (XRD). XRD result confirms a structural phase transition from bcc to fcc was occurring around 30% of Ni concentration in the alloy. Martensitic phase transition as well as a rigid peak shift was observed and reported in this paper. Such rigid shift in the reflections to higher angles could be due to the lattice contraction upon Ni substitution.

K1-0008

Influence of Suction/Blowing on MHD Fluid Flow over a Stretching Surface in a Porous Medium with Thermal Radiation

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Abstract. This paper investigates the characteristics of an unsteady two-dimensional boundary layer flow of a magnetohydrodynamic (MHD) fluid over a permeable stretching surface within a porous medium, considering the effects of thermal radiation and variable surface heat flux. Mathematical modelling is employed, leading to a set of coupled non-linear ordinary differential equations through similarity transformations. Numerical solutions are obtained by using shooting method combined with the fourth order Runge-Kutta algorithm. The study explores the impact of dimensionless governing parameters on velocity and temperature profiles. The findings reveal that as the permeability parameter and suction parameter increase, there is a corresponding increase in the skin-friction coefficient. Conversely, when blowing is introduced, the opposite effect is observed. Additionally, higher suction parameters lead to a reduction in both momentum and thermal boundary layer thicknesses. The results provide valuable insights into fluid dynamics in this context and offer practical implications for related engineering applications.

Viability Detection of Soybean Seeds using α-variogram based Statistical Analysis Sadhana Tiwari ^{1,2}, Reena Disawal¹, Mahendra Singh Thakur¹, Shivangi Bande² and Amit Chatterjee^{1,a)}

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Abstract. Biospeckle patterns are observed in a specimen with temporal variations due to physiological, biological or chemical activity. For biospeckle pattern analysis, various point-based and intensity-based methods were proposed in the past. These techniques involve manual selection of region of interest and have variation in activity index due to different parameters such as number of frames, nature of specimen, correlation, etc. To circumvent these drawbacks of conventional methods, α -variogram based statistical analysis was recently introduced. In this work, we investigated the applicability of α -variogram based analysis for viability detection of soybean seeds. Several seed specimens were irradiated and acquired using biospeckle apparatus. Acquired images were then processed using statistical analysis. From the obtained results, strategy was conclusively established as accurate and computationally efficient for soybean seed viability detection.

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A2-0004

Fusion Probability for a Pair of Particles in Inertial Confinement Fusion

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Abstract. This study aims to model the probability of fusion of two particles in inertial confinement fusion. When the separation between two particles (D+ and T+ in this case) becomes zero, they combine to form He and release a neutron. When T+ approaches D+ the probability density of the approaching particle decreases due to presence of the potential of the second. The probability of fusion of the two particles is said to be the same as the probability of the approaching particle when its separation with the resting particle becomes zero. This study models the fall in probability density of the approaching particle and uses it to determine the probability of fusion between the two particles.

Gamma Ray Energy Interaction Parameter of Mass Attenuation Coefficients and Exposure Build-up Factor of Alkaloids

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Abstract: The parameters of energy such as partial interaction cross section and total attenuation coefficients (µtot.) of Ephedrine (EPH) (C₁₀H₁₅NO) and Adrenaline (ADR) (C₉H₁₃O₃N) are calculated by using the 'WinXcom' computer software over the energy range 1 KeV to 100 GeV. In this study regularities of interaction of gamma radiation with Ephedrine (EPH) and Adrenaline (ADR) such as the exponential attenuation law, the decrease of the mass attenuation coefficient with increasing energy of gamma quanta, the increase of the mass attenuation coefficient with increasing atomic number of the absorber and the proportionality of the mass attenuation coefficient corresponding to Compton scattering to the atomic number of the absorber are discussed. Geometric progression (GP) method was used to calculate gamma-ray energy exposure buildup factors (EBF) of taken samples for the energy range 0.015-15 MeV, and penetration depths upto 40mfp. The result suggests that the interaction processes are 'Z' dependent. The graphs and equations describing the above dependency currently enable in determining the density of various taking Ephedrine (EPH) and Adrenaline (ADR). The values of EBF were found to be smaller in lower and higher photon energy regions whereas very large in intermediate energy region where Compton scattering dominates. Here ADR has higher values of $\mu_{\text{(total)}}$ in energy range as compared to EPH, so ADR shows good shielding effectiveness for gamma rays.

A2-0006

Ionization Cross Sections for Purine Nucleobase (C₅H₅N₅) Due to Electron Impact Manoj Kumar*¹ and Rajeev Kumar²

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Abstract: Electron interaction with biomolecules, such as DNA and RNA, in particular electron attachment (dissociative) studies have achieved prominence with the pioneering work of Sanche and coworkers. The low energy ionization radiation (9-20 eV) interactions with living cells produces various damages in DNA and RNA such as single-strand breaks, double-strand breaks, base deletions etc. Electron impact ionization of biological importance molecules plays a vital role in radiation damage and therapy. In the present study, we have calculated the total ionization cross sections for Adenine ($C_5H_5N_5$) a purine nucleobase molecule with biological importance, by electron impact in the incident electron energy range from ionization potential to 2 keV by employing a well-established Jain-Khare semiempirical approach based on Bethe and Möllor cross sections. In the absence of experimental data, the present theoretical results for total ionization cross sections are in satisfactory agreement qualitatively as well as quantitatively with available theoretical results are presented.

Impact of Allura Red-AC Photosensitizer Azo Dye In Photogalvanic Solar Cell For Solar Power Generation And Storage

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Abstract: Dye sensitized Photogalvanic solar cells (DSPSCs) are a photovoltaic energy conversion system due to their low cost, ability to fabrication on various substrates, structural modifications, easily transparency, photovoltaic output and its potential applications in wearable devices, energy sustainable buildings, solar-powered windows, etc. In this regard for conversion of solar energy into electrical energy we use DSPSC devices consist of Allura Red-AC, Ascorbic Acid and Sodim laurylsulphate reagents as photosensitizer, reductant and surfactant respectively. The photopotential, photocurrent, power at power point, fill factor (η), conversion efficiency and cell performance (t_{0.5}) at light intensity 10.4 mWcm⁻² have been studied of the order of 920.0 mV, 760 μA, 144.54 μW, 0.2067, 1.38% and 110 minutes respectively. Surfactant are used to increase conversion efficiency and storage capacity. The impact of various parameters like concentration of Azo dye, reductant and surfactant, variation of pH, light intensity and diffusion path length were observed at different conditions.

A2-0008

FFT Predicated ECG Steganography Utilizing Pixel Pair Procedure: A Procedure for Securing Patient Private Information

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Abstract. In the current time we are observing an expansion is the way how the data is available to the society and the people around the globe. Around the Globe with the advent of new connectivative technology the threat of the data having its stolen has gone to a great level. So, the need of the hour is to find out ways to provide privacy to the private data. WBAN known as Wireless Body Area Network is an emerging technology and in this paper is a foundation stone for the problem that is the Health care problem. WBAN is having a wide number of application platforms. The current paper is on the monitoring of Remote Healthcare Monitoring. There are several parameters associated with a Human being like ECG, Heart Rate and Blood Pressure which could be monitored remotely and in turn give rise to an implementation of a Remote healthcare monitoring system. In the current scenario again privacy or security of the data is a vital issue. The paper focuses on the ECG steganography method for providing security in the health monitoring application. The way implemented is giving away by which authentication as well as confidentiality of the data related to the patient is done and the basic purpose is solved as well.

The Characterization of Pure and Market Honey Using Dielectric and Spectroscopic Methods

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Abstract: - The Microwave X-Band Bench technique was used to test the dielectric characteristics of pure and market honey at a frequency of 8.735 GHz. Market honey samples had a higher dielectric loss, loss tangent, and penetration depth at room temperature and lower dielectric constant value than pure honey. These dielectric properties suggest that the microwave-based dielectric characteristic might be used to forecast the presence of sugar owing to adulteration processes. In FTIR band range of 4000-400 cm-1 was used to determine the existence of C - C functional groups for D-glucose and fructose. It is associated with the transmission region that examined the concentrations of sugars including glucose, fructose, and sucrose in samples of pure and market honey at various intensities. Samples S2 and S3 have different intensities at 920 cm⁻¹,983 cm⁻¹ and 965 cm-1, indicating varying glucose and fructose content. The presence of adulteration in market honey can be predicted using lower intensities which signify reduced enzyme activity. The dielectric and spectroscopy approaches may be used to detect the impacts of adulteration.

A2-0010

Molecular Docking Study of Binding of Perylene Di-imide to a Bio Molecular Human Telomeric G-quadruplex

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Abstract. Human telomeres are comprised of d(TTAGGG) repeats involved in the formation of G-quadruplex DNA structures. Ligands stabilizing these G-quadruplex DNA structures are potential inhibitors of the cancer cell-associated enzyme telomerase. In human cells, telomerase adds multiple copies of the 5'-GGTTAG-3' motif to the end of the G-strand of the telomere and in the majority of tumor cells it results over-expressed. Several structural studies have revealed a diversity of topologies for telomeric quadruplexes, which are sensitive to the nature of the cations present, to the flanking sequences, and probably also to concentration, as confirmed by the different conformations deposited in the Protein Data Bank (PDB). The existence of different polymorphism in the DNA quadruplex and the absence of a uniquely precise binding site give rise to check docking approach. As target we have selected six different experimental models of the human telomeric sequence d[AG3(T2AG3)3] based on three G-tetrads and as ligands the perylene di-imide. We checked out molecular docking simulation of binding of perylene di-imide to a slected G-quadruplex using dock 6.9 to examine whether or not to reproduced the loop binding mode of perylene di-imide. The simulation gave the two highest rank docking pose of perylene di-imide and the binding mode were external stacking on the terminal guanine tetrade and the groove binding.

Antibacterial activity of Entada phaseoloides Saponin on Escherichia Coli

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Abstract. Entada phaseoloides holds significant importance in oriental remedies. For a long, the plant has been used in addressing conditions such as rheumatism, backaches, leg pain, sprains, jaundice, malnutrition-induced edema, and bruises and it stands as one of the most extensively utilized plants in contemporary times. In the present work, we have carried out an experimental study to investigate the impact of saponin extracted from En- tada phaseoloides on E. Coli. For this, we first extracted the saponin of the plant from solvent extraction procedures using a soxhlet apparatus and performed microbial tests on the sample. The E. Coli growth inhibition revealed mild antibacterial activity of the saponin.

A2-0012

Phytofabricated Silver Nanoparticle-Modified Glass Electrodes for Non-Enzymatic Potentiometric Urea Sensing

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Abstract. Global demand for milk is increasing with population growth, but industry ethics are a concern due to profit-driven practices. In this work, a surface-active electrode composite was synthesized using a surface-modified Corning glass electrode (TiO2-LL@AgNPs) coated with phytofabricated silver nanoparticles from Leucaena leucocephala leaf extracts. To investigate the structural properties of the phytofabricated silver nanoparticles, various characterization techniques were used, including scanning and transmission electron microscopy (TEM), UV-visible, X-ray diffraction (XRD), Fourier transform infrared (FTIR), and energy-dispersive X-ray (EDX) spectroscopy. The findings revealed the synthesis of crystalline, spherical silver nanoparticles with an average size of 11.93 nm and a maximum absorption of 436 nm. This surface-modified electrode was made from synthesized silver nanoparticles and used for the electrochemical detection of urea in both artificial samples and real milk. The detection was based on the measurement of the induced potential resulting from the surface interaction between urea and the developed electrode. The composite was successfully used for urea detection. The sensing parameters, including the sensing range $(5.0 \times 10^{-6} \, \mathrm{M})$ to 25.0×10^{-6} M), sensitivity (2.50 mV μ M⁻¹ cm⁻²), and detection limit (2.48× 10^{-6} M). The developed electrode exhibited a response time of 5 minutes and maintained stability for 28 days. This environmentally friendly sensor is comparable to the spectroscopic approach and shows minimal interference from other substances present in milk.

Capture contribution in very low energy (e, 2e) process on H

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Abstract. The triple differential cross section (TDCS) for the single ionization of hydrogen negative ion and helium atom at excess energy of 8eV is calculated and compared to each other in the equal sharing energy and $\theta_{ab} = 180^{\circ}$ using distorted-wave Born approximation. Post collision interaction (PCI) is incorporated through effective charge model. The spin state of the exchange electron is taken care of. The capture process is found to be quite contributory for hydrogen negative ion rather than helium atom.

B2-0003

Generation Of Firehose Instability By Injection Of Hot Electron In The Magnetosphere Of Jupiter

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Abstract. In this paper firehose instability has been generated by injection of hot electron beam in the magnetosphere of Jupiter for loss cone generalized distribution using kinetic approach. The effect of temperature anisotropy and ratio of number density of hot and cold electrons has been studied. In the generalized distribution loss-cone distribution index j=0 (Bi-Maxwellian) is considered as a cold background and j=1 (loss-cone) is for hot electron injection. After using computer technique growth rate for fire hose instability has been calculated in the Jupiter magnetosphere at $R_j=17$.

Synthesis and Characterization of Organic Non-Linear Optic Active Material: An Experimental and Theoretical Approach

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Abstract. In this work, a potential organic nonlinear optical single crystals of methyl(2E)-2-{[N-(2formylphenyl) (4-methylbenzene) sulfonamido] methyl}-3-[4-(propan-2-yl) phenyl] prop-2-enoate (M2N2F4MS4P) were obtained by slow evaporation technique using an ethyl acetate solution as a solvent and characterized by single crystal XRD, FT-IR and NMR in the solid phase. The compound M2N2F4MS4P belongs to triclinic system with the space group P^{-1} with cell constants: a = 10.9242(8)Å, b = 11.0613(6) Å, c = 11.7893(6) Å, $\alpha = 106.168(2)^{\circ}$, $\beta = 92.764(3)^{\circ}$, $\gamma = 111.045(2)^{\circ}$, V = 1259.39(13) Å³ in the unit cell. The structural and electronic properties of M2N2F4MS4P are computed using DFT/B3LYP/6-311G++ (d,p) method by Gaussian 09W program. In the crystal, molecules are coupled through intermolecular C-H π interactions making a one-dimensional supramolecular network along (110). A meticulous molecular image and intermolecular interactions proceeding from charge delocalization and hyper conjugative interactions of the molecule were analyzed with NBO analysis. The HOMO-LUMO energy gap, Mulliken, thermodynamic properties and NLO properties were theoretically predicted. The Hirshfeld surface investigation was done to explore intermolecular interactions and connected two-dimensional fingerprint map, enlightening the comparative influence of those interactions within the crystal structure quantitatively. The SHG efficiency of the grown material is found to be 2.62 times the reference material. Overall, the properties advise that the present material may be an efficient candidate for optoelectronic devices.

B2-0005

Comparative Study of Nonlinear Dynamic Behavior of Perfectly Balanced Horizontal Rotor and Vertical Rotor Supported by Tilting Pad Journal Bearings by Computing Frequency Response

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a) Corresponding author: harsh.dixit29346@paruluniversity.ac.in, b) tcgupta.mech@mnit.ac.in **Abstract.** The nonlinear dynamic analysis has been carried out to investigate the dynamic behavior of a perfectly balanced horizontal rotor (HR)-tilting pad journal bearing (TPJB) system and perfectly balanced vertical rotor (VR)- tilting pad journal bearing (TPJB) system by computing frequency response of both the systems. To do so, governing differential equations (GDEs) of motion for HR-TPJB system and VR-TPJB system has been derived and they were solved by finite element method (FEM). The GDE of motion of both systems have been combined to form a unit set. This unit set represents the HR/VR-TPJB system. Implementation of computational numerical integration technique has been employed to solve equations of motion of both the systems which has been solved using the MATLAB® ODE-15s solver. Indigenous MATLAB® program has been created to compute the above-mentioned frequency response of the system efficiently. Time-Amplitude Response and Frequency-Amplitude Response with Phase at both the TPJB's and rigid disc locations have been computed by Fast Fourier Transform (FFT). The dynamic behavior of the perfectly balanced HR-TPJB and VR-TPJB systems have been analyzed for different rotor speeds. The results and discussions on the nonlinear dynamic behavior of perfectly balanced HR-TPJB and VR-TPJB systems operating at low and high rotor speed have been explained which indicates HR-disc is more unstable than HRjournal inside identical 4-pad TPJBs at low rotational speed (1500 rpm). The frequency response of both HR-TPJB system and VR-TPJB system at low speed (1500 rpm) shows that peak amplitude appeared much before in VR than HR, which indicates even in low rotational speed, VR-TPJB system is more unstable than HR-TPJB system. Results demonstrated that the balanced VR operated at high

speed (6000 rpm) is more prone to instabilities than its horizontal counterpart (HR-TPJB system) at the same speed (6000 rpm).

B2-0006

Impurity identification in an ultracold gas of bosons atoms in phase-space

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Abstract. In recently, we have proposed a scheme to sensitive quantum measurement using ultracold atoms [Phys. Lett A **453**, 128484 (2022)]. Most attractive properties of the system, its measurement sensitivity limit is very high due to the quantum nature of the ultracold atoms. Here, we propose a temperature sensitivity measurement of the order of Pico-Kelvin and an another sensitive measurement of purity gas of bosons in phase-space. The impurity in the gases changes the effective mass of the system; this combined mass is the reduced mass. This mass difference will results in relative phase difference which we measured in Wigner phase-space. In this scheme we showed a measurement when mass difference is 2.4 % of actual mass.

B2-0007

Quantum Chemical Calculations of 4-(4-Nitro-Phenoxymethyl)-benzo[h]chromin-2-one (NM2BC) Using Density Functional Theory (DFT)

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Abstract. Coumarin and its derivatives are belonging to the class of heterocyclic compounds having their wide range of applications in biology and medicine. 4-(4-Nitro-Phenoxymethyl)-benzo[h]chromin-2-one (NM2BC) belongs to the class of coumarin. In the present study, the molecular geometry is optimized at B3LYP/6-311G level using Gaussian-16 software through density functional theory (DFT) approximations. The Frontier Molecular orbitals (HOMO and LUMO), Molecular electrostatic potential (MEP), Non-linear optical properties (NLO) and Natural bonding orbitals (NBO) are studied. The FMO studies revealed that the HOMO-LUMO energy gap of the NM2BC is 3.37eV. The MEP mapping infers the preferential electrophilic and nucleophilic binding sites in the titled molecule. NLO calculation confirmed that the titled molecule is promising candidate to lighten the NLO based application. The second order perturbations of Fock-Matrix in NBO analysis are incorporated in the estimation of most possible intensive intramolecular interactions.

Fusion analysis of ¹⁹F + ⁹³Nb system at sub-barrier energies

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Abstract. The fusion dynamics of reaction $^{19}\text{F} + ^{93}\text{Nb}$ is analyzed by applying simple Wong formula and symmetric asymmetric Gaussian barrier distribution (SAGBD) model. For this reaction, Wong calculation agrees with fusion data at energies lying above the Coulomb barrier but fails to explain the data specifically at energies below barrier. This divergence in results shows importance of internal degrees of freedom associated with the colliding nuclei. In SAGBD model, a Gaussian type of weighted function is employed to explore the effect of nuclear structure on fusion cross-sections and the effect of coupling is determined in terms of model parameters λ and V_{CBRED} . The estimated values of these parameters are considerably large, which further reflect involvement of nuclear structure properties of colliding nuclei in fusion process.

B2-0010

Structural Study of Ga-doped Garnet (Li7La3Zr2O12) Solid Electrolyte with the help of Rietveld Refinement

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Abstract. The Ga-doped Li₇La₃Zr₂O₁₂ (LLZO) Solid State Electrolyte (SSE) has been looked in with the help of X-ray diffraction and its structure has been successfully refined by the Rietveld method. The SSE crystallizes in the Li_{6.55}Ga_{0.15}La₃Zr₂O₁₂ phase with cubic space group number 220 and unit cell parameter 13.0029 Å, and La₂(Zr₂O₇) phase with cubic space group number 227 and unit cell parameter 10.8128 Å. With 109 total reflections, the structural parameters of both the phases conversed to R_p = 15.5, R_{exp} = 10.51, R_{wp} = 20.8, and the goodness of fit i.e. χ^2 was obtained as 3.91. The core of the Liion migration channel has been defined as the loop formed by the Li32, Li1, Li2, and Li22 sites with minimal Li...Li distance and occupational disordering of the Ga-doped LLZO SSE. The electron density plots of Li_{6.55}Ga_{0.15}La₃Zr₂O₁₂ phase have shown maximum electron distribution inside the unit cell for lanthanum atoms.

Double Differential Electron Ionization Cross Sections of CF₂Cl₂ Molecule

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Abstract. In this paper, the first time we have investigated double differential ionization cross sections (DDCS) of CF₂Cl₂ molecule and its fragments using the Jain-Khare semi-empirical method due to electron impact, which is relevant to multiple calculative purposes to understand the fundamental characteristics of CF₂Cl₂ molecule. For Double differential cross-sections, there are no comparable results to compare the current calculated findings related to the CF₂Cl₂ molecule; however, the calculated data may be used as reference data for future purposes.

B2-0012

Numerical Investigation on the Effect of various ETLs and HTLs on the Performance of an Improved, Stable MAPbI3 Perovskite Solar Cell with a PbS QD Layer: Using SETFOS 5.3

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Abstract. Perovskite solar cells (PSC) can be considered potential competitors of silicon solar cells owing to their excellent photo conversion efficiency (PCE). However, this has not been possible so far in view of its poor environmental stability. A layer of quantum dot (QD) can improve the stability as per earlier reports. We, thus modelled and optimized the PSC device performance using Lead Sulphide QDs along with methyl ammonium lead iodide (MAPbI₃) as the absorber, taking the effect of various materials as HTL (NiO, P3HT, Spiro-MeOTAD and PEDOT: PSS) and ETL (C₆₀, PCBM, TiO₂ and ZnO) using SETFOS. In addition, the impact of layer thicknesses, doping concentrations of absorber layers along with optimized HTL/ETL as well as temperature, on the photovoltaic parameters, including PCE, are also thoroughly investigated. The optimized device obtained has a configuration of ITO/Spiro-MeOTAD/MAPbI₃/PbS/ZnO/Ag with an open circuit voltage of 1.022914 V, a short circuit current density of 27.39669 mA/cm², fill factor of 88.3114 %, a power conversion efficiency of 24.73963% and an external quantum efficiency of 90.504%. The results of this investigation shall gain increasing scientific interest in future and conjointly find applications in the design of more stable, low-cost, efficient SCs based on QD's and perovskite materials.

Thermoelectric Properties of The B1 And B2 Phases of BaO

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Abstract. Thermoelectric properties of barium oxide crystallizing in the B1 and B2 phase are investigated. After achieving the ground state of the crystal, the band structure calculations are interfaced with the Boltzmann transport equations to unveil thermoelectric properties. We have found the Seebeck coefficient, power factor and electrical conductivity. The effect of temperature is also studied. The existing experimental and theoretical data are in accord with all of the present findings. It is found that B1 crystal behaves as a good thermoelectric material at high temperature. It shows n-type conductivity. The B2 crystal also shows n-type conductivity but its behavior as a good thermoelectric material is observed at low as well as high temperature.

B2-0014

A Proton Transfer Study Using Density Functional Theory

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Abstract. Imidazole is an organic colorless compound having chemical formula $C_3H_4N_2$. It produces a slightly alkaline solution when dissolved in water. Imidazole is included in many biological molecules. The fundamental one is amino acid histidine which contains an amino group, a carboxylic acid group and a positively charged imidazole functional group. Histidine plays an important role in structure and binding functions of hemoglobin. Consequently, to investigate its proton transfer property becomes essential. In this study proton transfer from imidazole to chloranil is studied by Density Functional Theory.

Double Differential Electron Ionization Cross Sections of CF₂Cl₂ Molecule

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Abstract. In this paper, the first time we have investigated double differential ionization cross sections (DDCS) of CF₂Cl₂ molecule and its fragments using the Jain-Khare semi-empirical method due to electron impact, which is relevant to multiple calculative purposes to understand the fundamental characteristics of CF₂Cl₂ molecule. For Double differential cross-sections, there are no comparable results to compare the current calculated findings related to the CF₂Cl₂ molecule; however, the calculated data may be used as reference data for future purposes.

B2-0016

Effect of point defects and lattice distortions on structural, electronic and magnetic properties of Co₂MnAl Heusler alloy

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Abstract. Using the first-principles calculations within density functional theory, we have investigated the influence of various points defects (i.e., antisite disorder and vacancy defects) and lattice distortions on the structural, electronic, and magnetic properties of Co2MnAl alloy. For antisite disorder, we have considered the different binary antisite disorder viz; Co(Mn), Co(Al), Mn(Co), Mn(Al), Al(Co), Al(Mn) with disorder degrees upto 12.50%. Here, A(B) disorder represents the B atom replaced by the A atom, which maintains the same number of atoms in supercell. For vacancies, mono- and di-vacancies for Co, Mn and Al have been considered. All point defects have been modeled using a 64-atom supercell. Meanwhile, cubic strain and tetragonal distortion have been considered using the 16-atom unit cell for the lattice distortions. From our calculation, the Mn-poor structure resulting from the Al(Mn) disorder is most likely to be found due to its lowest formation energy, while the Al-poor structure resulting from Co(Al) and Mn(Al) antisite disorder has the highest formation energies; therefore they are less likely to be found. Besides, the spin polarization (P) increased from 75% to 100% for the Co(Al) and Mn(Al) defects, while the Co(Mn) defect is responsible for the dramatic decrease in spin polarization. Other antisite disorders show marginal effects on the P and maintain a high spin polarization of 70% - 80%. Also, the total spin magnetic moment (Ms) is immune and nearly identical for the rest of the considered disordered structures. For all types of antisite disorder, the disorder effect is localized, with changes in P and M_S primarily driven by the disordered atom. In contrast, all kinds of vacancy defects resulted in a significant reduction in both P and M_S, with the most pronounced changes observed in the case of Mn vacancies. Unlike antisite disorder, the effects of vacancy defects were not localized and extended beyond the nearest neighbouring atoms. Turning to lattice distortion, for the cubic strained structure, we found that a uniformly strained structure with a volume change of \pm 5% is likely to exist in real samples due to low relative energy differences ($\leq 0.1 \text{ eV/f.u.}$). The density of state (DOS) shape and Ms are unchanged due to the same crystallography of lattice, while the spin polarization decreased linearly with increasing the cell size due to the shifting of Fermi level w.r.t. the cell volume. In the case of tetragonal distortion, distorted structure has very high relative energy and, therefore, is less probable to occur. DOS shape changes due to the reduce symmetry of the system, resulting in the arbitrary changes in P and Ms. These findings would be helpful for the material design using Co2MnAl for the spintronics applications.

Quark-Hadron Phase Transition in Pb+Pb Collisions

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Abstract. The focus of the analysis has been to examine pseudo-rapidity distributions obtained for the γ -like particles in pre-shower photon multiplicity detector. Heavy ion collisions with nuclei at relativistic energies are ideal to create an environment with large nuclear and energy densities. Such a situation is quite suitable for the formation of a deconfined state of matter known as hot Quark-Gluon Plasma (QGP) which subsequently cools and expands. In this process the energy density becomes high enough so as a phase transition Quark-Gluon Plasma (QGP) to hadrons state occurs The results are compared with simulation analysis using VENUS event generator. In this study an attempt is made to understand phase transition in the domain of conventional statistical physics according to Ginzburg-Landau Model.

B2-0018

Numerical Analysis of Thermo-Mechanical Behaviour in Friction Stir Welding of Al/Mg joints

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Abstract. As the demand for proficient dissimilar material joining methodologies escalates, Friction Stir Welding (FSW) has emerged as a prominent solid-state welding technique. This manuscript presents a comprehensive numerical analysis of the thermo-mechanical behaviour during the FSW of Al/Mg joints. The study employs a fully coupled thermo- mechanical analysis to explore the intricate interplay between heat generation and mechanical response. The Johnson-Cook model is utilized to capture the material behaviour under high strain-rate conditions typical of FSW. The investigation delves into temperature distribution, heat transfer, and residual stresses. Notably, temperature disparities between the advancing and retreating sides are observed. The analysis highlights the influence of tool rotation and traverse speeds on residual stresses. The insights gained from this numerical investigation contribute to a better understanding of FSW and its optimization for Al/Mg joint welding.

A comparative study of extraordinary and ordinary modes in self-focusing of higher order modes of elegant hermite cosh-Gaussian laser beams in an collisionless magnetized plasma

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Abstract. In present investigation, Three-dimensional cosh-Gaussian laser beam is introduced. The self-focusing and defocusing of elegant hermite cosh-Gaussian laser beam in collision less magnetized plasma have been investigated theoretically. The final Differential equation for the beam width parameter is derived by following Wentzel-Kramers-Brillouin (WKB) and paraxial approximation through standard Akhmanov's parabolic wave equation. The final results of numerical computation are presented in the plot of beam width parameters $(f_1 \& f_2)$ versus normalized propagation distance (ζ) . In present investigation the author shows nonlinear effect due to different modes, magnetic field (B_0) and decentered parameter (b) on self-focusing and defocusing in collision less magnetized plasma. The results show well enhancement in beam of self-focusing.

B2-0020

First Principles study of structural, electronic and elastic properties of bulk silicon, germanium and α -tin

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Abstract. First principles calculations based on density functional theory (DFT) are performed to investigate the structural, electronic and elastic properties of bulk silicon, germanium and α -tin using Quantum ESPRESSO package under Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA). Calculated equilibrium lattice constant for Si (5.47Å), Ge (5.77Å) and α -Sn (6.66Å), bulk modulus of bulk Si (87.5GPa), Ge (57.1GPa) and α -Sn (35.6GPa) has well agreement with experimental results. The electronic band structure shows silicon is indirect band gap material while germanium and α -tin are direct band gap material.

Computational Studies on Oxidative Mechanism of Nirtrate Reductase

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Abstract. The reduction of nitrate to nitrite is the important reaction in nitrogen cycle that has been carried out by metallo-enzymes that has unique non-standard metal-dithiolene cofactor in active site with Mo/W at the centre. The oxidation reactions mechanism have been studied using DFT methods inorder to understand the most favorable reaction pathway with Mo and W at the centre. The studies will suggest the plausible reaction pathways and the effect of centre metal atoms in the nitrate to nitrite conversion.

B2-0022

Transport properties of Rare Earth Nitrides: Semi-classical Boltzmann theory Ranju Bala^{1, a)}

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Abstract. The transport properties of the rare-earth nitrides DyN, ErN, HoN, ScN and YN have been calculated from 50K up to 800K. The transport parameters of the rare-earth nitrides were evaluated by using the semi-classical Boltzmann theory based on the calculated band structure. The charge carrier concentration and the electrical conductivity linearly is found to increases with increasing value of temperature and is in agreement with the experimental work. The value of electrical conductivity for HoN, ScN, YN, DyN, ErN from 50K up to 800K range was evaluated and plotted, ErN was found to have heighest electrical conductivity at the same temperature as compared to others. Seebeck coefficients for ErN, HoN, ScN, YN at 50K to 800 K were evaluated. It was found that Seebeck coefficients for ErN, HoN, ScN increases linearly as the temperature increases. Slope of increase of seebeck coefficients with increasing temperature was found highest in case of HoN. A linear plateau was also observed in the Seebeck coefficients plot of YN at the temperatures above room temperature. The thermal electronic conductivity of rare-earth nitrides as a function of temperature is calculated and plotted for the temperature range of 50K to 800K. It is observed that at low temperatures ke is zero, as temperature increases the ke increases exponentially in agreement with the experimental data. As the temperature increases, the electronic thermal conductivity increases exponentially, in agreement with the experimental data.

Thermoelectric properties of Zintl phase compound NaBaSb

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Abstract: Thermoelectric properties of Zintl phase compound NaBaSb are explored through first principles calculations. The compound NaBaSb exists in hexagonal crystal structure. The band structure with DOS is shown in Fig.1(a) and DOS using PBE and MBJ functionals. From Fig. it is clear that the band gap using PBE and MBJ are 0.68 eV and 0.41 eV respectively making this compound suitable for thermoelectric applications as they require narrow band gaps.

B2-0024

Predicting Composition and Bulk Modulus Property Linkage Using Materials Informatics Dharani $M^{1,a)}$ and Praveen $M^{2,\ b)}$

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Abstract. The combined application of informatics and material science is explored. The data containing 83989 compositions are extracted from Materials database and after cleansing the extracted data, the linkage between composition and the bulk modulus property are predicted with the technique of Composition Based Feature Vector (CBFV) by using suitable Classical Machine Learning Algorithms and further with a Deep neural network.

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Quantum States of Ultracold Bosons in Optical Lattices Interacting via Long-range Interaction Rohit Panda^{1, a)} and Budhaditya Chatterjee^{2, b)}

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Abstract. We simulate a one-dimensional system of a few ultracold bosons trapped in an optical lattice with long-range interactions from an ab initio perspective using the MCTDH-B method. We emphasize the distinct influence of the long-range interactions and the effects not observed by systems with contact interactions. We consider both the nearest neighbor and the next-nearest neighbor interactions in addition to the usual contact interactions. We observe and analyze the ground state that arises due to the intricate interplay between the interaction potentials and the non-trivial influence of the particle number. By systematically tuning the coupling between different interaction types and varying particle numbers across different regimes, we uncover a diverse set of novel ground-state configurations whose emergence is governed by the delicate interplay of competing energetic factors.

B2-0026

Topological nodal line features in semimetal LiYGe

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Abstract. The field of topology in condensed matter physics has generated a lot of interest during the past decade because of their rich novel physics. The topological quantum materials have dragged the attention of worldwide researchers not only due to their exotic transport properties but also their possible applications in quantum computing etc. Three types of semimetals in the field of topology are discovered namely, Dirac semimetals, Weyl semimetals and nodal line semimetals. The topological properties of LiYGe compound are explored through first principles calculations. Nodal lines can cross the Brillouin zone (BZ) in the shape of a closed ring or a line. The nodal line compound LiYGe exists in hexagonal structure.

Theoretical Investigation of Li/Na Adsorption on Nitrogen-Doped Armchair Graphene Nanoribbons

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Abstract. In this study, interaction of Li/Na with N-doped armchair graphene nanoribbon (AGNR) has been studied by using density functional theory. The effect of nitrogen doping of AGNR on the adsorption of Li/Na has been studied by calculating adsorption energies and binding distances. Pristine AGNR is not suitable for adsorption of Li/Na atoms as their adsorption energies on pristine AGNR are smaller than the cohesive energies of bulk Li/Na. It has been found that adsorption strength of Li on N-doped AGNR gets enhanced as compared to pristine AGNR and adsorption energy of Li is greater than the cohesive energy of bulk Li. On the other hand, N-doping improves the adsorption abilities of AGNR but adsorption energy of Na is smaller than the cohesive energy of bulk Na. Thus, N-doped AGNR can be considered suitable for the adsorption of Li. Further, electronic structure analysis of pristine and N-doped AGNR shows that semiconducting nature of pristine AGNR turns into metallic upon the adsorption of Li while N-doped AGNR remains metallic in nature before and after the adsorption of Li atom.

B2-0028

The conformation of duplex DNA assimilates intermediate-state of B-DNA and A-DNA to accommodate R-TFO to form R-triplex

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Abstract. DNA triplexes form during the initiation of several vital processes such as replication, transcription and homologous recombination in natural cells. These triplexes are not same as most widespread Hoogsteen triplexes. Hoogsteen triplexes need A-form of DNA for the accommodation of its TFO (triplex-forming oligonucleotide) but the natural environment doesn't provide A-DNA so frankly. Therefore it is thought that some other type of triplexes such as R-triplexes (Recombinant triplexes) may form during these processes. To examine the conformation of duplex DNA in R-triplex, we designed an R-triplex using mixed ATGC sequence of DNA. The structure was equilibrated and a molecular dynamics simulation of 150 ns has been done. To study the structure of duplex DNA the trajectories were analyzed. After the study we found that the conformation duplex DNA deviates in such a way that it is now able to accommodate a natural single strand DNA using same sequence of first strand of duplex DNA. We also found that the structure of duplex DNA of R-triplex is not exact as B-DNA but it is intermediate structure of B-DNA and A-DNA.

Sputtering Yield and Surface Composition Analysis of Metal Targets under Ar, Xe and Self Ion Impact

Nargis

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Abstract. Energy loss processes of an energetic ion impact inside target materials are described via electronic energy loss (Se) and nuclear energy loss (Sn). When the ion velocity reaches close to the Bohr velocity of the target electrons, it transfers its energy to the electrons through inelastic collisions, leading to excitation, and a fraction of its energy is transferred to the target nuclei by electron-phonon coupling. As the ion traverses deeper, its velocity decreases, and the energy is transferred to the target nuclei through elastic scattering, leading to atomic displacements and defect creation. These modify the material properties depending upon beam energy, fluence and incident angle. Patterning of arranged surface structures has emerged as an established top-down method to fabricate precisely located nanostructures of well- controlled sizes and shapes for numerous potential applications in storage devices, nano-crystallites and templated fabrication of various nanostructures.

Analysis of surface atomic composition and sputtering yield is done for metal targets (Al, Co, Ni, Ag Au, and Cu) using the computational program SDTrimSP. These metals undergo surface morphological changes upon keV ion radiation, as reported in various experimental studies. A detailed investigation of variation in sputtering yield with the fluence is done for Ar, Xe and self-ion impacts on these metals.

B2-0030

GIS-based assessment of Physico-chemical Parameters and Metal contamination of groundwater: A Case study of Hapur (Uttar Pradesh)

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Abstract. The aim of this study was to assess the quality of groundwater in Hapur by examining various physico-chemical parameters, including pH, Electrical Conductivity (EC), Total Dissolved Solids (TDS), Total Hardness (TH), and heavy metal contamination (such as Al, As, B, Ba, Cd, Cr, Hg, Mn, Ni, Pb, Se, Sr, and Cu). Samples were collected from four different sites in Hapur, and a combination of groundwater sampling, chemical analysis, and Geographical Information System (GIS) was employed to achieve the research objective. Arc-GIS was utilized to analyse the spatial distribution of water quality parameters in the selected areas. The analysis of metal contamination was conducted using the inductively coupled plasma-optical emission spectroscopy (ICP-OES) technique. The obtained results were compared with the standard values set by the World Health Organization (WHO) and the Bureau of Indian Standards (BIS). The spatial study revealed that EC, pH, TH, and TDS exceeded the permissible limits defined by WHO. The pH values indicated that the groundwater in the study area was alkaline. Moreover, metals such as Ni, Mn, Hg, and Sb were found to exceed the WHO limits in the majority of the samples. Based on these findings, it is crucial to identify specific geographic areas to develop effective plans for groundwater resource management. Additionally, raising awareness among individuals responsible for polluting or contaminating groundwater is essential. The importance of water quality should be emphasized to ensure better protection and preservation of this vital resource.

Device Modelling and Numerical Simulation Study on Reduced Graphene Oxide as HTL in PTB7:PC71BM Based Organic Solar Cell

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Abstract. Organic photovoltaic cells (OPV) seems to be the emerging solution to renewable energy devices due to its extraordinary features, namely flexibility, semi-transparency, solution processing capability, and low cost. Research on graphene derivatives such as reduced-graphene oxide (rGO) as hole transport layer (HTL) for high-performance OPV have been intensely growing due to their unique electronic properties. work, numerical simulation In this Au/rGO/PTB7:PC71BM/PFNBr/FTO has been done using SCPAS1D software. We have optimized the characteristic parameters of the PTB7:PC71BM (active layer), rGO (hole transport layer) and PFN-Br (electron transport layer). The proposed solar cell gave an enhanced efficiency of 12.84% with fill factor of 61.20%, Voc of 0.8047V and Jsc of 26.025793mA/cm². The influence of intensity of sunlight is studied by varying the intensity from 1 to 5 sun. And the effect of temperature on device performance is also investigated by varying the temperature from 253 to 333 K. Our simulation studies show that the proposed organic cell provides the best output in its class at 1.5 sun and 333 K.

B2-0032

Design of Dual Port Electromagnetic Planar Sensor based on Single Split Ring Topology

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Abstract. In this paper, a simple geometry of sensor is proposed based on split ring structure, by considering the manufacturing simplicity with error free sensing. The dual port electromagnetic planar (DPEP) sensor is designed to operate at 2.4 GHz using Rogers RT/duroid substrate with relative permittivity ϵr =2.2, $\tan\delta$ =0.0009 of height h=1.6 mm. The sensor is designed for the characterization of lossless materials by estimating their relative permittivity. It is dual port sensor, hence transmission response is observed for material characterization. The characterization of lossless material is done by observing the resonance frequency shift with varying relative permittivity of material under test (MUT). This sensor shows appreciable results in sensing a wide range of dielectric material i.e., ϵr =1-80. The effect of height (H) of superstrate on the resonance of the sensor is analysed using parametric analysis. The proposed sensor can be prominently useful for material characterization and for the determination of soil moisture content.

Polarizability of some Cobaltocene, Nickelocene, Derivatives Using Empirical Approach

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Abstract. The molecular polarizabilities of 20 cobaltocene derivatives have been calculated using a new empirical approach based on the square of the sum of the atomic hybrid components (ahc), namely $\alpha(ahc) = \frac{4}{N} \left(\Sigma_A \tau_A \right) (\mathring{A})^3$. Where the summation proceeds over all atoms A=1,2,3,upto N, and N is the total number of electrons in the molecule. Common trends and patterns of behavior are recognized and discussed. The results have been compared with those calculated by using Lippincott & Stutman's method.

B2-0034

Designing and Simulation of a Terahertz Frequency Filter Based on SIS Stub Waveguide Coupled with a Split Ring Resonator

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Abstract. We propose a tunable filter composed of a semiconductor-insulator-semiconductor (SIS) stub waveguide with a split ring resonator (srr) at terahertz(THz) frequency. Indium Antimonide (InSb) is selected as the semiconductor and air as the insulator. The electromagnetic energy is carried through the propagating surface plasmons through the S-I interface and coupled to srr placed at one side of the stub waveguide. The transmission studies of the proposed structure have been done using the finite element method and obtained symmetric mode and antisymmetric mode resonances. The device can be used for filtering THz frequency within the range of 0.2THz to 1.2 THz by varying the structural parameters. The effective mode index ($N_{\rm eff}$) and propagation constant calculations are done for the fundamental mode to obtain the height of the stub waveguide. The symmetric mode shows more sensitive variations in the resonance according to the change in parameters. The simulated structure is a promising candidate for an integrated optical circuit and terahertz devices as a filter and also can be used for sensing applications.

Double Differential Ionization Cross-Sections of a CF₃Cl Molecule by Electron Impact Using a Semi-empirical Approach

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Abstract: We evaluate the partial and total double differential ionization cross-sections (DDCS) of a CF₃Cl molecule by electron impact using a modified Jain-Khare semi-empirical approach. We evaluate the double differential ionization cross-section as a function of energy loss of primary electron or secondary electron energies at fixed incident angles (30° and 60°) and fixed incident electron energies, i.e., 100, 200 and 500 eV. Angular variation of DDCS at fixed incident electron energies and fixed secondary electron energies are also being evaluated. No other data for double differential ionization cross-sections are available for comparison.

B2-0037

MIMO Based Radio-over-Fiber link for Millimeter Wave Generation Using External Optical Modulator

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Abstract. In this paper, photonically assisted millimeter wave signal generation techniques are proposed for modern space applications. For this, two designs are investigated with different optical modulators, namely, amplitude modulator and Dual Drive-Mach Zehnder Modulator (DD-MZM). A 2*2 Wavelength Division Multiplexing (WDM) transmitter with a 100 GHz frequency spacing is used to broadcast Multiple-Input Multiple-Output (MIMO) signals, and it encodes the signals using a 1Gbps pseudo-random bit sequence with return-to-zero coding. The Electrical Constellation Visualizer is used to examine the distortion in the proposed Radio over Fiber (RoF) links. The opti-system software simulation for DD-MZM design confirms a high-frequency millimeter wave signal with 60 dBm optical sideband suppression ratio (OSSR) and radio-frequency spurious suppression ratio (RFSSR) 72 dBm. Whereas Amplitude Modulator based architecture produces mm-wave signals with high Q-factor and low loss. Therefore, the merging of MIMO and RoF technology is a better solution for generating mm-wave signals for next-generation communication systems.

C2-0001

MIL-101(Fe)-NH₂ with Polyethylenimines Metal Organic Frameworks based Mixed Matrix Membranes for CO₂ Capture and Gas Separation Applications

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Abstract. MIL-101(Fe) based MOF particles were successfully synthesized and modified with amine functional groups. Briefly, 6.18g of 2- aminoterephthalic acid and 20.25g of FeCl3.6H2O were dissolved in 450 cm³ of DMF (N, N'-dimethylformamide). The reaction was carried out in an autoclave by sealing the above mixture and heated at 110 °C for 20 hr. After that, the sample was cooled to room temperature and filtered for final product by washing multiple times with DMF and ethanol. The unreacted species present in the pores were removed by overnight extraction using ethanol as solvent. Further, the final product was oven dried for overnight at 80 °C. To study of chemical composition, morphology of these materials with various techniques such as XRD, SEM, TEM, TGA and DSC etc. were performed. The elemental analysis of the prepared MIL-101(Fe)-NH2 product was found as C, 38.35%; H, 1.98%; N, 5.61% whereas for MIL-101(Fe)-NH2 (Fe3Cl1C24H14N3O13, 756.38 g/mol) is C, 38.11%; H, 2.00%; N, 5.56%. 500 mg of methanol exchanged MIL-101(Fe)-NH2 was activated by heating in oven for 2 hr at 100 °C. Afterwards, the activated material was dispersed in 15 cm³ methanol in a glass vial. The opening of the glass vial was fitted with a rubber septum, while the reaction system was evacuated using a vacuum pump, and nitrogen was introduced into the system. This process was repeated for three times to remove all the air from the system, and further reactions took place in inert nitrogen atmosphere. Subsequently, the PEI solution containing 50 wt% water was added to the dispersed material to achieve 10, 25, 35, 50,75, and 100 wt% PEI vs MIL-101(Fe)-NH2. The mentioned proportions were prepared with different number of PEI-X monomer units (X= 800, 1200, and 2000). The suspensions were stirred for 24 hr at ambient temperature. Subsequently, the glass vials contained reaction mixtures were shifted to preheated oven at 60 °C and dried overnight at same temperature. Then the samples were collected and grinded and the samples were noted as MIL-101(Fe)-NH2-PEI-X-Y (X=800, 1200, 2000; Y=10,25, 35, 50, 75). The as synthesized pure and modified MOF particles were introduced into the polymer matrix to fabricate mixed matrix membrane via solution casting method. Briefly, the polymer was dissolved in solvent by continuous stirring followed by the addition of MOF fillers in step wise with ultrasonication to avoid the agglomeration of MOF particles in the solution. Further stirring was carried out to obtain homogenous dispersion of the particles in the solution. Then the solution was casted on petri dish and allowed for drying to evaporate the solvent present. Finally, after complete drying the resulting membrane was termed as MMM. To optimum the stability of the membranes, MOF/Polymer membrane composites with different thicknesses were prepared. These MMM were used for permeability and selectivity measurement of with different gases as H2, O2, N2 and CO2. Further photocatalytic CO2 capture in synthesized MOFs and polymer based composite membranes was measured under visible/solar light irradiation.

C2-0002

Gd₂O₃@g-C₃N₄ Impregnated Polypyrrole is Amply Intercalated for Superlative Super-Capacitive Performance

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Abstract. Supercapacitors are suitable for energy storage devices due to their quick charging and discharging rates and high cycle life. However, due to their poor energy density, supercapacitors cannot entirely replace batteries. A novel series of Gd₂O₃/gC₃N₄@PPy (GGP) nanocomposite (NC) for rare earth metals was produced by sonication and in-situ polymerization. By using cyclic voltammetry (CV), galvanostatic charge discharge (GCD), and electrochemical impedance spectroscopy in 1 M H₂SO₄, the electrochemical application of synthesized nanocomposites was carried out (EIS). This synthesized series was delineated through the use of Fourier transform infrared (FTIR), ultraviolet spectroscopy (UV), Brunauer-Emmett-Teller (BET), thermal gravimetric analysis (TGA), and X-ray diffraction, this synthesized series was defined (XRD). Using techniques for field emission scanning electron microscopy, the NCs' morphology was assessed (FESEM). When examined electrochemically for super-capacitive characteristics, the composite in this series with the best performance was 0.6g g-C₃N₄@0.3g Gd₂O3 impregnated PPy (GGP2). With a specific capacitance of 1189.18 F/g at a current density of 1 A/g and a larger capacitive holding of 96.6 percent after 10,000 charging and discharging loops, it obtained the highest value and is therefore well suited for super-capacitive performances. Due to its straightforward synthesis, huge specific capacitance, improved energy density, and recyclable nature, GGP is a strong contender for usage as an energy storage technology.

D2-0001

Structural features, emission analysis, and Covalency comparison of Neodymium acylpyrazolone complexes using Oscillator strengths, covalency and Judd-Ofelt parameters Maitrey Travadi and R. N. Jadeja*

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Abstract. Three distorted square antiprismatic eight coordinated Neodymium acylpyrazolone complexes NdL₁, NdL₂, and NdL₃ were synthesized having the composition [Nd(L)₃(H₂O)(EtOH)]. Utilizing ESI-mass, FT-IR, single crystal x-ray diffraction, and thermogravimetric methods, the structure of all three complexes were examined. ${}^4G_{5/2} \leftarrow {}^4I_{9/2}$ transition in electronic spectra exhibits hypersensitivity. Through a comparative analysis of calculated oscillator strength, Judd-Ofelt parameters, rms deviation, radiative lifetime and covalency parameters in various solvents, hypersensitivity, symmetry characteristics, and covalency have been thoroughly investigated. The promotion of 4f-4f electric-dipole intensity has been found to be particularly successful with ethanol, pyridine, DMF, and DMSO. Utilizing Judd-Ofelt Ω_4 values and Hirshfeld analysis, long-range secondary $\pi \cdots \pi$ stacking or H-bonding interactions were investigated. Using solid-state emission spectra, intensity of emission spectra and antenna effect energy diagram was examined.

D2-0002

Dual wavelength excitable novel phosphor for applications in cognitive therapy and display devices

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Abstract. Ca₂La₂O₅:Eu³⁺ (x=0.5 to 2.5 mol%), a novel color-tunable phosphor, has been successfully synthesised employing a modified solid state reaction process using a chemical flux. Ca₂La₂O₅:Eu³⁺ is an uncommon novel dual-wavelength excitable phosphor because of its broad absorption spectrum, which spans in the range of 250-600 nm. It exhibits broad white (400-650 nm), red (627 nm) photoluminescence (PL), which were attributed to one or more ${}^5D_0-{}^7F_J$ (J =1-4) transitions of the Eu³⁺ ion, respectively. After gradually raising the concentration of the Eu³⁺ ion, an effective energy transfer between La3+ and Eu3+ was noticed. Images obtained using scanning electron microscopy showed elongated rod-like formations with a 2.0 um average diameter. The white (0.41, 0.35), red (0.62, 0.38) zones were discovered to have the chromaticity coordinates (x, y) positioned with the excitable wavelengths of 395 nm, and 467 nm, respectively. Additionally, the temperature-dependent luminescence spectra of Ca₂La₂O₅:Eu³⁺ excited at 467 nm was investigated. It displayed good thermal stability, and at 150 °C, photoluminescence intensity was about 73% of the room temperature. The activation energy was estimated mathematically to be 0.19 eV. The outcomes show that the phosphor is appropriate for LED applications like cognitive therapy due to its 627 nm emissions and also display device applications for its dominating red component in w-LEDs, which are otherwise challenging to achieve in single-component systems.

D2-0003

Universality in Dipolar Ising Model

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Abstract. The behaviour of many magnetic and dielectric solids composed of rare-earth elements and transition metals and the more contemporary magnetic super-lattices, is governed by dipolar interactions. They are anisotropic and long ranged, and arise from nuclear magnetic moments in alkali hydrides and solid ³He, electron magnetic moments in rare-earth fluorides, chlorides, and hydroxides, electric dipole moments in ferroelectric and antiferroelectric structures, etc. As a consequence, such systems have various states ranging from ground states with complicated magnetic order to the presence of glassy dynamics characterized by a plethora of relaxation times. These systems are well-captured by the dipolar Ising model (DIM) with nearest-neighbour exchange interactions and long-range dipolar interactions. Depending on the relative interaction strength there are four phases of distinct magnetic order and symmetry. Using Monte Carlo simulations, we perform deep quenches to study domain growth. This important non-equilibrium phenomenon has not been addressed as dipolar interactions are notoriously difficult to handle theoretically. Our study reveals that, in spite of the anisotropy in interactions and diversity in ground state configurations, there is universality in the ordering dynamics of all phases.

Exploring New Aspects With Attenuation Coefficient As Parameter To Mark Sensitivity of G.M. Detector

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Abstract. This article aims to explore the sensitivity of the functioning of the G.M. counter toward the operating voltage. The accuracy and precision of the G.M. Counter depends highly on the accurate choice of operating voltage. We here extracted the values of dead time at different values of operating voltage. The large dead time value will hinder the detection of the radiation. The lesser value of dead time in G.M. counter means the more actual measurement of radiation. However, the dead time measurement depends on the choice of operating voltage. We hereby showcased the drawback of a detection system by measuring its dead time variation with operating voltage. We also showcased the sensitivity of G.M. Tube through variation in operating voltage. We explored this aspect through a quantitative study on the basis of radiation counts attenuated for Iron and Lead plates

E2-0002

The comparative study of hybrid vehicles with traditional vehicles

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Abstract. The economy growth and progress of a nation are significantly influenced by public and private transportation. Market expansion and market sturdiness are made possible by an efficient transportation infrastructure. It supports and facilitates the robust economic expansion that results in increased global competitiveness. The less productivity and a loss of social connections are all major factors of inefficient systems. This study presents the comparative study of various hybrid electric vehicles (HEV). The elaborative studies of literature survey have been carried out to meet the research objective.

Capture contribution in very low energy (e, 2e) process on H

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Abstract. The triple differential cross section (TDCS) for the single ionization of hydrogen negative ion and helium atom at excess energy of 8eV is calculated and compared to each other in the equal sharing energy and $\theta_{ab} = 180^{\circ}$ using distorted-wave Born approximation. Post collision interaction (PCI) is incorporated through effective charge model. The spin state of the exchange electron is taken care of. The capture process is found to be quite contributory for hydrogen negative ion rather than helium atom.

E2-0004

Exploring the Potential of Exascale Computing: Advancements and Implications

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Abstract. Exascale Computing is the high performance computing system that can measure quintillion calculations per second. It is capable to perform the calculations of 10¹⁸ Floating Point operations (FLOPS) per second. It is the term given to the next 50-100 times increased speed over very fast super computers used today. High performance computing application helps to simulate large scale application, machine learning, artificial intelligence, Industrial IoT, weather forecasting, healthcare industries and many more. The increased computational power will enable researchers to tackle more complex problems, collects and analyse larger data sets, perform simulations with high accuracy and resolutions. Exascale computing has the power to transform scientific research, spur innovation, and tackle complex issues that were previously computationally impractical. This paper describes a brief description, architecture and various applications of exascale computing such as healthcare, microbiome analysis, etc. This paper also presents the future and research aspects of Exascale Computing.

Study of Electromagnetic Ion Cyclotron wave for ring distribution with magnetic model in Jovian Magnetosphere

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Abstract. The analysis based on observations by Ulysess of Electromagnetic Ion Cyclotron (EMIC) wave in Jovian magnetosphere has been done in this paper. In Jovian's magnetosphere it has been observed that there are various types of large frequency radio emissions by the mechanism of resonant interaction. This paper we have considered the phenomenon of wave-particle interactions between EMIC wave along the magnetic field lines and fully ionized magnetospheric plasma particles with parallel propagation of wave which evaluates the elaborated dispersion relation for ring distribution finding also with and without magnetic field model. Using the method of characteristics solution and kinetic approach, expression of growth rate has been derived. Following a parametric examination of the plasma's temperature anisotropy, thermal velocity, and number density, the impact of these variables on growth rate was examined using graphs.

E2-0006

Examining Approaches To Image Segmentation in Medical Image Analysis

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Abstract. Accurate segmentation of medical images is required to make the correct diagnosis. This article provides a comprehensive overview of the various successful strategies for producing exact segmentation. Despite this, assembling certain components in a timely manner can be difficult. The adaptive technique of image segmentation could be used to handle a variety of computer vision challenges. A variety of segmentation approaches are reviewed and analysed in this article. The findings of this study can be used to identify when and how to employ image segmentation techniques, as well as to improve their efficacy and accuracy. Image processing comprises several subfields, some of which include object representation, analysis, and data visualization. Segmenting an image is a critical first step in each of these subfields. An image is segmented so that it can be broken into pieces that can be used to meet the needs of a certain application. Manual segmentation is time-consuming and often unnecessary in ordinary situations. This implies that when automatic algorithms fail, human or semi-automated segmentation methods can be used instead.

Experimental Study of Viscosity and Capillary Flow of Liquid

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Abstract. A water solution is allowed to flow under gravity through a horizontal capillary tube of uniform bore and small area of cross section. The water molecules in contact with the wall of the capillary tube are at rest, and those along the axis of the tube flow with a maximum speed. This difference in the movement of water molecules from one layer to the next inside the capillary tube resists the flow of water due to molecular friction of the liquid known as viscosity. The flow of water solution from one end to another of the horizontal capillary tube is due to a difference in pressure at the two ends. We perform an experiment to measure the coefficient of viscosity η and the resistance R of flow of water solution for different concentrations c using Poiseuille's viscosity apparatus.

E2-0008

Exploration of Δ baryon resonances in the realm of Reggephenomenology

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Abstract. The current article is concentrated on the spectroscopic investigation of the Δ baryon, which contains only up (u) or/and down (d) quarks. The orbitally and radially excited state masses are obtained by employing the phenomenological approach, the Regge theory. Various relations are extracted between Regge slope, intercept, and baryon masses with the assumption of quasi-linear Regge trajectories. With the aid of these relations, the resonance masses of Δ baryon are evaluated with the suitable spin and parity quantum numbers of all the states. The obtained mass spectra is compared with the experimental observations and also with the outcomes of various theoretical approaches. In addition to the mass spectra, the Regge trajectories are constructed in the (J, M²) and (n, M²) planes.

Analytical Study of Electromagnetic Ion cyclotron for ring distribution with an A.C electric field in the magnetosphere of Jupiter

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Abstract. In this paper, an analysis of electromagnetic ion cyclotron waves in the magnetosphere of Jupiter at 17 Rj has been done based on observations made by Ulysses. In the magnetosphere of Jupiter, due to the mechanism of resonant interaction, it has been observed that there are various types of large frequency radio emissions. The phenomenon we have considered in this paper is the wave-particle interactions between the fully ionized magnetosphere and electromagnetic ion cyclotron waves along magnetic field lines has been taken with the parallel propagation of wave to evaluate the detailed dispersion relation with ring distribution in the presence of AC electric field in collision-less magnetosphere of Jupiter 17Rj.

E2-0010

All Charm Tetraquark Spectra In Coulombic Plus Quadratic potential

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Abstract. A non-relativistic model with relativistic corrections is used to generate the mass spectra of all charm tetraquark in the diquark-antidiquark system. Fitting parameters are derived by numerically solving the Schrodinger equation for the charmonium "meson using the coulombic potential and the harmonic confinement interaction potential. The mass spectra of all charm tetraquark is calculated in present work by systematically reducing a four-body problem to a two-body problem using the parameters obtained from charmonium spectra.

Preparation and effect of additives n-ZnO doped p-NiO Screen printed thick films on Structural and Electrical Properties

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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 static gas sensing system. 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 are reported. The prepared thick films of ZnO doped NiO nanoparticles were analysed for electrical parameters namely TCR, activation energy and sheet resistivity, specific surface area were evaluated at different concentration of zinc oxide that assured the prepared material has a semiconducting nature. Electrical characterization results resistivity decreases from 6283.377 to 1972.727 with increase in wt.% concentration of ZnO. Such a prepared film can be used in fabrication of optoelectronic devices.

E2-0012

Exploring the Ξ_b' with baryon in context of new experimental results

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Abstract. In the present study, singly bottom baryon Ξ_b' has been studied. We used Hyper Central Constituent Quark Model (hCQM) to make calculations for the masses of the ground state and excited state of Ξ_b' . In this model we employed higher order correction such as second-order correction in the mass, within the context of spin-dependent terms, enables us to accurately observe the correct order of spin splitting. We determine spin-parity J^P for ground and excited states Ξ_b' baryon. We determine the property, such as the magnetic moment of the ground state of Ξ_b' , and compare it with other theoretical approaches.

Performance of a Different types of Grid Connected Wind Generators: a Comparative Study

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Abstract. Now a days, the major of our energy requirements have fulfilling through conventional energy sources. Many options are available in conventional energy sources, from which thermal power plant-coal based plays a major role. But as it causes the adverse effect on the nature, it is essential to adopt alternative sources which are better in the performance. So, the renewable sources or non-conventional are now moving forward, out of all renewable energy sources wind plays a vital role as it is most cost effective energy source used for power generation & to fulfil our demands. By considering the challenges & difficulties to be faced with interconnected wind power systems using different generators, it is very essential to study the various types of wind generator systems and their impact on the power generation as they affect to the power quality issues. In this paper, the recently used generators & some newer concepts has been studied. The doubly fed induction generator, Brushless doubly fed reluctance generator and the Switched reluctance generator are viable alternatives for wind power applications.

E2-0014

Symmetrised Basis Functions for the water molecule using the Eigenfunction Method G. Gnanasangeetha

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Abstract. In this work we have shown the construction of irreducible basis using the Eigenfunction Method (EFM) for the class operators of the C_{2v} symmetry group, taking H_2O molecule as a specific example. The EFM is introduced as the theory of discrete symmetric groups for molecular systems in exact analogy to Lie's theory of continuous symmetric groups, a founding stone for obtaining non-degenerate eigenstates of say Hydrogen atom in conjunction with Dirac's principle of Complete Set of Commuting Operators. From the class operators a complete set of commuting operators are obtained by considering the regular representation of the H_2O molecule and calculations are presented using simple matrix algebra thereby demonstrating the merits and elegance of the EFM.

The study of Seawater Intrusion in Agricultural Soil using the Microwave X-band Band Bench, Absorption and Spectroscopic Methods

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Abstract. Seawater intrusion into agricultural land is a major problem due to global warming. To observe the effect of seawater on micronutrients in agricultural soil, we studied the dialectical and micronutrients behaviour of seawater-contaminated soil. The dielectric characteristics of soil samples were evaluated using the Automated Microwave X-Band Bench at a frequency of 9.55 GHz. Dielectric constant of soil is increasing with increasing distance from the sea face. A chemical method is implemented to study the variation in nitrogen, phosphorus, potassium (NPK) and sodium (Na). Using atomic absorption spectroscopy, micronutrients like Fe, Cu, Mn, and Zn were found. The dielectric constant shows a negative correlation with NK (nitrogen and potassium) and positive correlation to micronutrients. The mineral composition of soil was studied using FTIR in the band region of 4000-400 cm-1 and observed various mineral compositions, such as kaolinite, quartz, feldspar, carbonate, alum silicate at varying intensities. We correlated the study of variation in chemical composition and nutrients with dielectric constants and came to the conclusion that microwave-based dielectric characteristics can be utilized to predict the health of soil.

E2-0016

Study of Energy Levels for The Electronic Configurations 4p²4d, 4s²5d and of 4s² 6s in Kr-VI

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Abstract. Five times ionized krypton(Kr-VI) is a Ga-I like ion with ground state electronic configuration $4s^24p$. We have reported 20 energy levels of $4p^24d$, two levels of $4s^25d$ and one level of $4s^26s$. In this study we have considered previously reported levels of Kr-VI for the prediction of energy levels. The least square fitting of energy levels are made by using Cowan's quasi-relativistic Hartree-Fock code and the optimization of the energy levels are done by computational method LOPT.

A Progressive Study of Bessel Beams For Electron Acceleration

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Abstract. In the present work, we have explored Bessel beams and their properties for various application, particularly electron acceleration. Such beams exhibit some resistance to diffraction and are thus, a fantastic alternative to Gaussian beams. We have discussed optical trapping, material processing, free-space long-distance self-healing beams, optical coherence tomography, and other exciting applications based on these amazing beams. Also, the generation of Bessel beams using axicon lens is discussed in this paper. The incident plane wave tends to pass through an optical lens, an axicon, resulting in a zeroth order Bessel beam. We have utilized this lowest order Bessel beam for GeV electron energy gain.

E2-0018

Investigating the mass spectra of all bottom tetraquark in diquark-antidiquark formalism

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Abstract. Employing a non-relativistic model with relativistic mass corrections, exotic bound state tetraquark mass spectra is generated. Fitting parameters are calibrated by numerically solving the Schrodinger equation for the bottomonium meson using the coulombic potential and the harmonic confinement interaction potential in diquark-antidiquark system. Reducing a four-body problem in to a two-body problem using compact diquark with help of obtained fitting parameter, mass spectra of all bottom tetraquark is obatined.

Investigating the mass spectra of all bottom tetraquark in diquark-antidiquark formalism

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Abstract. Employing a non-relativistic model with relativistic mass corrections, exotic bound state tetraquark mass spectra is generated. Fitting parameters are calibrated by numerically solving the Schrodinger equation for the bottomonium meson using the coulombic potential and the harmonic confinement interaction potential in diquark-antidiquark system. Reducing a four-body problem in to a two-body problem using compact diquark with help of obtained fitting parameter, mass spectra of all bottom tetraquark is obatined.

E2-0020

Impact of periodic temporal variation of external harmonic trap on 1D quantum droplets

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Abstract. Recently, we have constructed an analytical model for investigating the dynamics of 1D quantum droplets (QDs) in presence of external harmonic trap utilizing 1D extended Gross-Pitäevskii equation (eGPE). We consider the mass balanced two-component Bose-Einstein condensate (BEC) mixture in which QDs are reported to stabilize under the comparable strength of effective repulsive interspecies mean field (EMF) interaction and attractive quadratic beyond-mean-field (BMF) interactions. The amplitude of EMF, BMF interactions and harmonic oscillator frequency emerged as key parameters for observing droplet to soliton transition in presence of external harmonic trap. Here, we observe the impact of periodic temporal variation of harmonic oscillator frequency on the dynamics of 1D QDs. The strength and frequency of periodic temporal and variation EMF/BMF controls the width/height of QDs. Further, we observe that the QDs to soliton transition and droplet fragmentation is connected with the amplitude of harmonic oscillator frequency, strength and frequency of temporal periodic perturbation.

Variable apodization method to reduce the effect of edge ringing of aberrated coherent optical systems

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Abstract. The coherent edge imaging of optical systems apodised with amplitude filters has been studied. Edge ringing can be appreciably mitigated using the chosen amplitude filters. The analytical studies were made for circular aperture. It is found that this type of apodization is more useful in reducing the ringing effect and also there is a perceptible increase in the edge gradient. Hence these amplitude filters are found to be effective in enhancing the resolving power aspects of edge imaging characteristics of optical systems.

E2-0022

Study of Decyl Glucoside – D-Fructose- Tartrazine System In Photogalvanic Cell For Solar Energy Conversion And Storage

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Abstract. Photogalvanic cell is type of photoelectrochemical cell based on Becquerel effect. A photogalvanic cell is a light-harvesting device used to convert solar energy into electricity and store it. In this work, the biodegradable surfactant Decyl glucoside was used because it helps solubilization and stability of the system, the synthetic dye Tartrazine acts as a photosensitizer, and fructose as a reducing agent acts as an electron donor. A very dilute solution of dye, reductant and surfactant has been used at high pH range in photogalvanic cell. Electrical parameters such as photopotential, photocurrent and power were studied. The current-voltage characteristic of the cell was also studied. The obtained V_{pp} , I_{pp} and P_{pp} of the cell are 864millivolt, $1050\mu A$ and $907.20\mu W$ respectively. The performance of the cell determined as $t_{0.5}$ is 205 minutes. Conversion efficiency of the PG cell is 8.723% and fill factor is 0.5543 for efficient photogalvanic cell in a sustainable manner.

Advanced Design Of Axial Rod Type Thermal Conductivity Measurement Setup

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Abstract. The objective of this work is to develop advanced design of Axial rod type experimental thermal conductivity setup with manual and automatic temperature measurement which is very much useful for research purpose as well as for the Post Graduate students to perform practical in laboratory and understand basic theoretical concepts. The developed set up is already in use for measurement of thermal conductivity for different types of solid materials and crystals. Various methods are used for the measurement of thermal conductivity. We have developed design of axial rod (Brass) type arrangement for steady state measurements. Suitable mechanical arrangement was fabricated for measurement of Top and Bottom temperature of the rod using J-type (Cr-Al) thermocouples. Special Heater with its power supply is designed to change the temperature manually at regular interval of time. The automatic measurement of temperature was also carried out by modifying the design which includes Thermocouple module and Arduino Nano Board. The corresponding measurement of temperatures at different points on Brass rod was carried out and corresponding thermal conductivity of crystal was calculated. Key pad is used to set the time for temperature display at regular interval of time in Minutes/Seconds in advanced design (which can be changed by program). Implications are discussed.

E2-0024

Theoretical Investigation of Probable Decay Modes in Potential Nuclei ^{296,297}Og, ²⁹⁷119, and ²⁹⁸120 for Future Experiments

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Abstract. Experimental research that focuses on adding new elements to the periodic table is continuing by several experimental facilities viz. Dubna laboratory: Russia, GSI: Germany, RIKEN: Japan, etc. The last synthesized element with proton number Z=118 and 10 new decay chains that were confirmed by several experiments. Some experimental works have also been performed to study the possibilities of synthesizing new elements with Z=119 and Z=120 by α -decay. In the last few decades, an exotic type of decay mode: cluster decay has also been theorized in the superheavy region. In the present work, we have studied probable decay modes viz. α -decay and cluster decay along with spontaneous fission in undetected and potential superheavy nuclei 296,297 Og, 297 119, and 298 120. We have applied the new modified Horoi formula (NMHF) formula to calculate α -decay half-lives, which is found to be more accurate in the superheavy region. To investigate other decay modes, spontaneous fission (SF) half-lives have been computed using the recently reported modified Bao formula (MBF), along with half-lives of cluster emission by using the modified BKAG (MBKAG) formula. After the comparison of half-lives of these different decays, the probability of α -decay has been found prominent, however, several heavy clusters viz. Kr, Rb, and Sr isotopes are also found with a finite probability of decay in this part of the periodic chart.

Biospeckle based automated method for seed type classification using machine learning

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Abstract. In present work, application of machine learning for biospeckle seed type classification is explored. Towards performing automated detection of seed type (Maize or Coffee), biospeckle features/signals are utilized. Several biosepeckle images of coffee and maize seeds are taken as specimen. Random forest based machine learning model was used for automated classification of different seed classification. For data splitting and model testing, label encoder and train-test split operation were performed. Finally, confusion matrix and accuracy score metric are utilized for evaluating performance of the learning model.

E2-0026

Effectiveness of Fractional Order PI Controller for Performance Enhancement of a Dynamical System

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Abstract. Fractional-Order-Proportional-Integral (FOPI) controllers have gained attention in recent years as an alternative to traditional Proportional-Integral (PI) controllers for improving the performance of dynamic systems. These controllers are based on fractional calculus, which extends the concept of differentiation and integration to non-integer orders. This paper concentrates on effectiveness of a FOPI controller in improving the performance of a dynamical system in terms of performance in terms of oscillation mitigation, improvement of the small-signal stability and stability margin. Fractional order controllers can provide more flexibility in tuning and can better adapt to complex and nonlinear systems. This often leads to improved control performance, especially in systems with unknown or time-varying dynamics. It helps to reduce steady-state error compared to integer order PI controllers. By adjusting the fractional order exponent, system's characteristics matched better with the controller's response. Also, the FOPI controllers allow for smoother transitions between different control modes or set points and helps to reduce overshoot and settling time in dynamical systems, as they allow for more precise control of the transient response. A simple test case of secondorder system has been taken into consideration in this work and then its state-model has been made for further investigation. The system has been examined under different operating conditions and found that the FOPI controller effectively improves the system response and worth it to append into a dynamics.

Design and Optimization of an LED based Optical Wireless Power Transmission System for Compact IOT Applications

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Abstract. Wireless power transmission (WPT) is the transmission of electrical energy, without cables connecting power source to targeted device, using electromagnetic field as a physical link. WPT brings great advantages of user convenience and operational flexibility for various applications such as charging mobile devices or flying drones. The WPT technologies can be classified into two categories, which are near-field (less than 1 meter) and long-distance (from 1 m to thousands of Kms) power transmission based on different applications. This article presents one of the long-distance techniques known as Optical wireless power transmission (OWPT). OWPT has been a promising solution for remote power supply, eliminating the need for batteries or power cables and electromagnetic interference. OWPT has outstanding features for highly efficient power transfer due to the unique characteristics of modern high-power LEDs like high directivity and energy concentration. In this work OWPT system is designed using an LED as light source, collimation and imaging lenses as light controlling optical elements and GaAs solar cell as the light to electrical energy converter. The designed OWPT system is optimized and simulated using ray-optics models at different Infrared radiation. The simulated irradiation power on the ray detector side is analyzed at 1 m and more than 1m distance from the LED source with different focal lengths of collimation Lense to predict optimum efficiency of the system.

E2-0028

Measurements of Neutron dose due to induced activity after using High energy Radiation in Linear accelerator

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Abstract. Neutron dose level due to induced activity after using high energy radiation near the treatment head has been measured with the help of the Neutron Dose Survey Meter (REM meter). Radiation Protection for the radiation worker is essential as they are coming in close proximity to the LINAC HEAD immediately after treatment delivery. This study was carried out to check neutron dose level 0.5m lateral from the Isocenter after using high energy radiation, around the gantry for field size of 5 cm x5 cm,10 cm x10 cm,20 cm x20 cm,40 cm x 40 cm with the variation of MUs 50,100,200,300,400,400,500, and 1000 MUs. The measured maximum instant reading for 15 MV 14.1msv/hr,10 MV 9.28msv/hr, 10FFF is 21 msv/hr at 0.5m lateral from the isocenter. This study indicates that at least 15sec min gap between two patient is necessary after using the high-energy radiation.

Existence and the Universe, what the Universe is made of and the Matrix representation of the Universe

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Abstract. In this paper, we first explore what is the phenomenon of "Being", and then we calculate the value of the quality of "Being" or "Existence". A derivation of the powers and states of "Existence" follows. Then we explain what the material cause of all things in the universe is or what it is made of. The material cause is surprisingly mathematical in nature. Then a theory is provided as to how the Universe originated from Nothing. Finally, an equation is derived which describes the state of the Universe at any given instant of time, which traces its origins from "Existence".

E2-0030

Dielectric Study of Polar -Polar Binary Liquid Mixtures

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Abstract. Present paper deals with study of microwave dielectric properties like dielectric constant, relaxation time, density for the binary mixtures of 2-propanol and water over the entire concentration range measured at 298K. The experimental data is further used to determine derived properties viz. Bruggman factor and the excess properties viz. excess static dielectric constant, excess viscosity, excess molar volume. The resulting excess parameters are used to indicate the presence of strong intermolecular interactions and strength of intermolecular interactions between the molecules in the binary mixtures.

Design and Optimization of an LED based Optical Wireless Power Transmission System for Compact IOT Applications

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Abstract. Wireless power transmission (WPT) is the transmission of electrical energy, without cables connecting power source to targeted device, using electromagnetic field as a physical link. WPT brings great advantages of user convenience and operational flexibility for various applications such as charging mobile devices or flying drones. The WPT technologies can be classified into two categories, which are near-field (less than 1 meter) and long-distance (from 1 m to thousands of Kms) power transmission based on different applications. This article presents one of the long-distance techniques known as Optical wireless power transmission (OWPT). OWPT has been a promising solution for remote power supply, eliminating the need for batteries or power cables and electromagnetic interference. OWPT has outstanding features for highly efficient power transfer due to the unique characteristics of modern high-power LEDs like high directivity and energy concentration. In this work OWPT system is designed using an LED as light source, collimation and imaging lenses as light controlling optical elements and GaAs solar cell as the light to electrical energy converter. The designed OWPT system is optimized and simulated using ray-optics models at different Infrared radiation. The simulated irradiation power on the ray detector side is analyzed at 1 m and more than 1m distance from the LED source with different focal lengths of collimation Lense to predict optimum efficiency of the system.

E2-0032

The effect of dust concentration on soliton reflection in an inhomogeneous plasma

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Abstract. In the present study, we examine a plasma characterized by its inhomogeneity, containing both trapped electrons and dust grains. Our study focuses on exploring potential modes within this plasma, their transformation into solitons, and the phenomenon of soliton reflection occurring at the density gradient. To understand these phenomena, we adapt the conventional Korteweg—de Vries (KdV) equation, which typically governs soliton behaviour, to accommodate the unique properties of this particular plasma. By identifying suitable transformations, we successfully solve this modified equation. In our investigation, we pay specific attention to the influence of dust charge and dust concentration in the presence of trapped electrons on soliton reflection. Notably, we observe that only the compressive solitons exhibit propagation and reflection within the plasma, albeit with a noticeable shift, under the condition that the dust charge density remains lower than the total charge density contributed by both types of electrons. We also explore how the propagation of a soliton in the plasma depends on the ion temperature.

Comparison of Direct Torque Control with PMSM vs DTC with Induction Motor Performance Suraj Karpe

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Abstract. Direct torque control is becoming into the industry norm for controlling the torque of induction motors. Based on the instantaneous torque and stator flux magnitude errors, as well as estimations of the flux location, a voltage vector is selected to limit the flux and torque errors within respective flux and torque hysteresis bands. Using Total Harmonic Distortion (THD), the electromagnetic torque, rotor speed, and stator current of DTC with PMSM and DTC with IM were effectively determined. DTC with PMSM decreased THD in torque, speed, and stator current by 12 percent when compared to DTC with IM [21]. This article makes use of the THD Minimization Switching Losses Minimization Technique. By minimizing switching losses, transistors are only switched when necessary to keep torque and flux within their hysteresis limits, leading to higher efficiency and reduced losses. Matlab SIMULINK has experimentally confirmed direct torque regulation with PMSM and IM.

E2-0034

Characteristics of Rectangular Microstrip Antenna and its performance for wireless communication.

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Abstract. In this paper presents a broadband microstrip patch antenna and performance for wireless communication. In basic form, a microstrip antenna consists of a radiating patch on one side of dielectric substrate which has a ground plane on the other side. It is generally made conducting materials such as copper or gold and can make any possible shape. For radiator, rectangular patch is used widely. This rectangular microstrip patch antenna is designed for wireless communication application. It works at 2.4 GHz with gain 12 dB for outdoor areas. It is also has a wide angle of beam in radiation pattern. Several advantages of such broadband antenna, such as planar, small in size, low cost, easy fabrication, simple structure and easy practical application. The motive of this paper, to achieve lower return loss, higher gain and lower VSWR (Voltage standing wave ratio). From simulation, the return loss, gain and VSWR were found to be – 13.89 dB, 6.6 dBi and 1.5 respectively. Inspite of this one main limitations with patch antenna is their narrowband performance due to its resonance nature. The results obtain that microstrip patch antenna can be used as client antenna in computer and workable antenna for wireless. There is still back lobe in radiation pattern of microstrip antenna.

Plasma Discharge Process In a Gun Type Plasma Device

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Abstract. In this communication we have reported the Paschen curve of argon plasma in a pulsed system where electrodes are placed in such a way that they are not parallel plate type. Here, the pulsed plasma is generated by using a washer plasma gun. The whole experiment is carried out in the CPS device. The working gas used is experimental grade argon. The Paschen curve obtained from such a system is analysed by comparing it with the Paschen curve obtained, using a parallel plate type electrodes. Anode material both for washer plasma gun and parallel plate type DC glow discharge device is copper. It is observed that the nature of Paschen curve for parallel plate type DC glow discharge device obeys the Paschen law as expected. However, the Paschen curve is modified when washer plasma gun is introduced in the CPS device by removing parallel plate type DC glow discharge device from it. It is worth noting that washer plasma gun is energised by a pulsed power supply. The pulse width of the voltage pulse here is 140µs. The minima of the experimental curve shifts towards higher value of pd in later case. Again, in the right branch of the said experimental curve for washer plasma gun discharge shifts towards x-axis (p.d axis) from that of the expected curve. Here p is base pressure and d is electrode separation.