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on

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About the Conference

Materials of different types, compositions, phases, sizes and properties are of importance for everyday uses. The tremendous demand for materials in a large variety of applications has led to the growing interest of the research community over the last few decades to study and design modern materials with improved performance. Such studies have contributed to the growth of Condensed Matter Physics (CMP) in a multidisciplinary nature. This field explores macroscopic and microscopic properties of matter experimentally, theoretically and computationally. The vast area of Condensed Matter Physics (CMP) research includes ideas from different disciplines such as Physics, Chemistry, Biology, Mathematics and Engineering. Being a primary subject of research and because of its global importance, Government of India runs various schemes to provide funding for basic research in CMP as well as for human resource and infrastructure development and international collaboration. These efforts have achieved tremendous success in publishing thousands of papers in journals of high repute and numerous patents within a very short period.

Advanced materials with useful properties can provide solutions in various sectors; such as cleaning water, obtaining healthy and hygienic food, designing sophisticated low-cost diagnostic equipment to prevent infant mortality, and malnutrition; technology for sensing and preventing environmental pollution; alternative harmless energy resources; self-reliance technology in security and safety sectors such as defence and anti-terrorism, etc. So, it is very exciting and fruitful to discuss the latest discoveries in terms of theory, technology, and applications of materials in the condensed phase.

The National Conference "Condensed Matter Days" (CMDAYS) aims to provide a suitable platform for young researchers and scientists to present their latest works on experimental, theoretical and computational condensed matter physics. The Department of Physics, Dibrugarh University is organizing the 32nd Edition of this conference (CMDAYS-2024) as part of the Diamond Jubilee celebration of the university. Following the general trend of CMDAYS, CMDAYS-2024 includes a wide variety of themes on emerging and interdisciplinary areas of condensed matter physics. The conference is expected to achieve a large gathering of the materials science community with ample thought-provoking ideas and discussions that will be helpful in the creation of sustained research collaborations.

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Keynote Address

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Keynote Address

Fluctuation-dominated Ordering

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Fluctuations and order are key concepts in statistical physics. Usually, they are thought to be antagonistic, as strong fluctuations often tend to destroy order.

However, this is not always so. Some systems show enormous fluctuations, despite which long-range order stays intact. In this talk, we will discuss states with fluctuation-dominated order, and several models and physical systems in which they arise.

Plenary Talk

Towards New Physics and Technology with Two-dimensional Materials

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It is exactly twenty years since one atomic layer of carbon, which we call graphene, was separated from graphite and shown that it could lead to a new generation of electronic field-effect transistors. Soon after, new forms of such 'two-dimensional' materials were discovered and led to a revolution that has now percolated to almost all conceivable sectors of technology, from electronics to health and environment, from composites to aviation, or from energy to quantum devices. Here, I shall talk about how the unique fundamental physics of graphene and its analogues led to the paradigm shift in several technologies, from electronics, opto-electronics and sensing, thermoelectricity, to neuromorphic designs. I shall emphasize the opportunity in designing new properties, probing fundamental concepts, and large-scale manufacturing, with this amazing class of two-dimensional solids.

Augmenting Molecular Imaging Efficiency based on Quantum Materials

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Motivated by prospective applications of contrast agents in next-generation molecular imaging technologies, this talk will provide a broad overview of current trends in molecular imaging and explore new perspectives. This wide ranging talk will touch on numerous applied problems related to the science of molecular imaging identifying the impact areas and materials challenges in contrast efficiency, diagnosis and imaging. Alongwith the development of new imaging modalities that need contrast agents or tracers for improved visualization, it is realized that nanoparticles can form an important class of materials with unique features suitable for biomedical imaging. In recent years, the notion of 'Quantum Materials' has emerged as a powerful unifying concept across diverse fields of science and engineering. The field has significantly expanded to encompass two-dimensional materials and their van der Waals heterostructures, Moire materials. It is my hope that this collective vision will contribute to sparking new fascinating questions and activities at the intersection of materials science, condensed matter physics, chemical engineering, and biomedicine.

Self-Assembly of Nano-patterns on the Surfaces: for Sensor, Device and Bio-Applications

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Ion Irradiation can produced an array of wonder materials. Low energy ion irradiation is especially suitable in fabricating a variety of nanostructures on the surfaces which show many important functional properties. We will present some results related to the development of Resistive memory Devices based on Oxide materials, Bio-applications with DNA and optical characteristics of Graphene Quantum Dots.

Special Talk

Superhydrophobic Surface: Self-cleaning or Superadhesion?

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Many water repellent surfaces are recognized as superhyrophobic surfaces where water contact angle attains ≥ 150^{o}. But whether the droplet will roll or slide over the surface, or stick to it profoundly depends on associated surface energy, microtexture, and composition. Spectacular roll-off based self-cleaning action can be witnessed *in lotus leaf, colocasia leaf* and similar systems. On the other hand, perfect pinning-based surface adhesion can be observed in case of *rose petals, hibiscus petals*, and similar natural entities. Interestingly, both the cases endorse very high WCAs, but it is the contact angle hysteresis (CAH) and three phase contact line (TCL) which decides the fate of the drop exhibiting either self-cleaning or superadhesion feature. The distinct phenomena will be discussed citing examples from nature.

Keywords: *Superhydrophobicity; adhesion; microtexture; roughness*

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Invited Talk

DFT Perspectives on Piezoelectricity Spin-orbitronics and in Selected Functional 2D Materials

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Novel properties such as piezoelectricity and valley physics arise at the nanoscale which are usually non-existent in the bulk form of the materials. HfN2 monolayers [1] exhibit valleytronic properties complementary to that in single-layer MoS2, while the merger of spin (valley) Hall effect with the Rashba effect is observed in h-NbN, h-TaN and monolayers screened via high throughput studies [2,3]. Out-of-plane piezoelectricity is induced at the interfaces of 2D semiconducting planar monolayers, which show in-plane piezoelectricity individually and zero out-of-plane polarization/piezoelectricity, such as GaN and boron monophosphide (BP) monolayers. The understanding reached in GaN/BP van der Waals heterobilayers (vdWHs) has been reinforced on MoS2/BP and MoSSe/BP vdWHs. Experimental verification of these theoretical predictions is encouraging. The origin of negative piezoelectricity at the interfaces of 2D dialkali oxide and chalcogenide monolayers has been elucidated [4] together with strain tunability in ultrahigh shear piezoelectricity in superflexible non–van der Waals graphitic ScX monolayers (X = P, As, Sb) [5]. 2D monolayers showing the simultaneous occurrence of ferroelectricity, ferroelasticity and large in-plane piezoelectricity will also be presented [6]. Last but not least, intrinsic carrier mobility estimation via several models in selected 2D materials will be discussed, as mobility plays a crucial role in determining the performance of electronic devices [7].

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Biomemristors as the Next Generation Memory Devices

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The implementation of biocompatible and biodegradable information storage would be a significant step towards next-generation green electronics. In this regard natural biomaterial and polymer-based Bio-memristors are very promising because of their sustainable, non-toxic, environment friendly, degradable and biocompatible properties. Such Bio-memristors possess excellent scalability, high flexibility, easy processing and low fabrication cost. A range of biomaterials like protein, enzyme, lipid as well as natural biomaterials directly extracted from plants or animals have been explored as active layers for memristor applications. In addition to sustainable solution towards e-waste, biomaterial based memristors may have fascinating applications towards nonvolatile memory, logic operation, implantable device, artificial synapse, artificial intelligence, transient electronics and so on.

In this lecture introduction about the ongoing research activities at our laboratory will be presented with a special emphasis on our ongoing work on biomaterials based Resistive Switching (RS) memory or bio-memristors.

RS memory is very emerging due to the simple device structure, fast operation speed, and long retention time etc. A typical RS memory cell consists of a simple electrode/active layer/electrode configuration. Generally, such devices can switch reversibly between high-resistance state (HRS) and low-resistance state (LRS) or among multiple resistance states under applied voltage bias.

Of late, we have designed and investigated a series of Bio-memristors using several biomolecules like protein, lipid as well as natural plant extract. Phospholipid DPPC and Protamine Sulfate (PS) showed biodegradable transient resistive memory suitable for WORM memory application. Noncytotoxic WORM Memory has been developed using Lysozyme with ultrahigh stability for transient and sustainable electronics. Plant extracts like Ipomea Carnea, rose petal, Water Lily etc have been explored for biodegradable and sustainable data storage as well as implantable device and neuromorphic computing applications.

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Mapping the Tricritical Point and Magnetostructural Quantum Phases of Columbites

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Transition metal oxides (TMOs) of the general formula $AB_2O_4/ABO_3/AB_2O_6$ (with A = TM, and B = Rare-earth or Nb/Ta) provide many unique fundamental physical phenomena at the atomic level which makes them richest families of magnetic materials [1-3]. Among such TMOs two systems with general chemical formula AB_2O_6 and AB_2O_3 are having peculiar importance in the field of microwave magnets and spintronics. The AB_2O_6 family usually crystallize in the orthorhombic crystal structure of columbite (Fig.1a) with four molecular formulae per unit cell except for $FeTa_2O_6$, $CoTa_2O_6$ and $NiTa_2O_6$ which crystallize into tetragonal (tri-rutile) crystal structure with two molecular formulae per unit cell. In these compounds usually A and B sites are occupied by divalent and pentavalent cations respectively, forming octahedra [AO_6 and BO_6] with six oxygen atoms. Columbites have potential applications in the field of satellite and mobile communications as dielectric resonators and filters, as electrochemical gas sensors, and in supercapacitors. In this direction, the present talk is focused on the exceptional magnetic properties of $MnNb_2O_6$, $CoNb_2O_6$ and $NiNb_2O_6$. The first half of the talk will be covering the mapping of the magneto-structural Quantum Phases of these columbites and realizing a Tricritical point on the H-T phase diagram (Fig. 1b). Striking features of such phase diagrams established from the magnetization measurements and heat-capacity data will be presented in the second part of the talk. The final part of the talk is concentrated on the field-induced spin-flop transitions exhibited by these systems together with the determination of the intrachain (*J*o) and interchain (*J*1 and *J*2)) exchange interactions of these compounds.

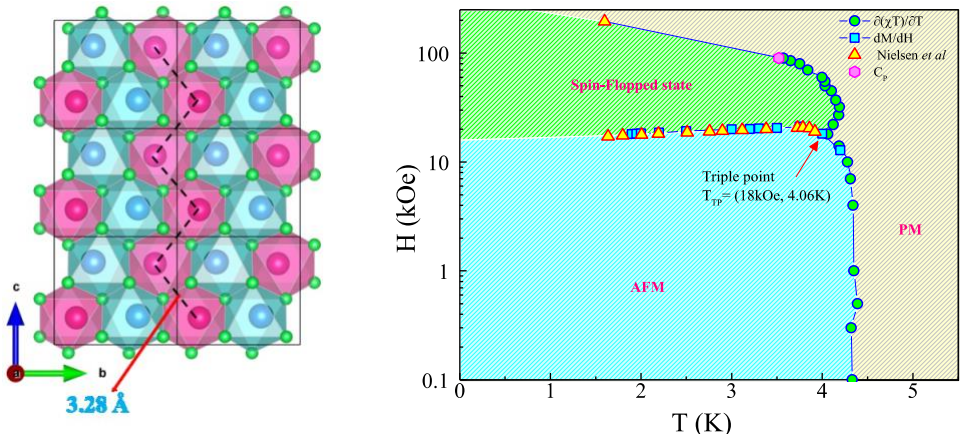

Fig. 1: (a) Typical schematic tri-rutile crystal structure of columbite (AB_2O_6). (b) Magnetic field –Temperature (H-T) phase diagram of $MnNb_2O_6$.

Keywords: Columbite, Spin-flop and Spin-flip spin-states, Crystal Phase Transition

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Enhanced Ferromagnetism in Ni-Doped Two-Dimensional Fe_5GeTe_2 Beyond Room Temperature Driven by Structural Distortions and Dynamical Electron Correlation

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Achieving beyond room-temperature ferromagnetism in two-dimensional (2D) magnets is immensely desirable for spintronic applications. Fe_5GeTe_2 is an exceptional van der Waals metallic ferromagnet due to its tunable physical properties and relatively higher Curie temperature (TC) than other 2D magnets. Using density functional theory combined with dynamical electron correlation and Monte Carlo simulations, we find that the TC of $(Fe_{1-\delta}Ni_\delta)_5GeTe_2$ monolayer can increase up to ~400 K at (δ: fractional occupation). Two specific Fe sublattices are identified to be the most energetically preferred sites to host Ni. Exchange interactions between particular Fe pairs play a dominating role in controlling TC, influenced by the dopant-induced structural distortions. Dynamical electron correlation induces site- and orbital-specific quasi-particle mass of Fe-*d* states with varying Ni concentrations. Our results agree well with the experimental observations on $(Fe_{1-\delta}Ni_\delta)_5GeTe_2$. This work provides fundamental insights into 2D magnetism as an interplay of structural and electronic aspects and would guide to tailoring exciting magnetic phenomena in similar systems.

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Nanocomposites from Lab Waste

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This presentation will discuss the conversion of lab waste to realize broadband photocatalysts having NIR-responsive transparent conducting oxide (TCO) nanocrystals integrated with p-type semiconductors. The discarded parts, which amount to two-thirds of the total mass of Al-doped ZnO (AZO) sputtering targets are converted to nano-phase AZO by the ball mill method efficiently. The blending of converted n-type AZO with p-type CuO or NiO is accomplished to enhance the catalytic elimination of environmental pollutants, especially, aqueous sulfamethazine and p-nitrophenol. The structural, morphological, and compositional attributes of the nanocomposites confirm the formation of polycrystalline nanograins of the individual phases. The AZO/CuO nanocomposite with optimum content (15 wt.%) of CuO stands as the most efficient broadband photocatalyst due to greater photosensitivity in a wider range extending from near-UV to NIR as a result of the combined effect arising from the wide band gap and plasmonic nature of AZO along with lower band gap of CuO. The degenerate AZO nanocrystals demonstrate surface plasmon resonance in the near-infrared reflectance spectra, which is supported by the simulation of the electric field enhancement due to the electromagnetic excitations. A mechanism of broadband light utilization in the charge carrier generation and separation leading to energetic redox reactions has been proposed in the contexts of the experimental findings complemented by the photoconductivity measurements. The speaker proposes to start with the science of aging stable AZO as the transparent conducting oxide and proceeds towards the central theme of high-yield conversion of lab waste to resources aiming at environmental remediation.

Keywords: Lab waste; AZO/CuO nanocomposite; Infrared plasmonics; Broadband photocatalysis

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Exploration of Helium Behavior in the Irradiation-induced γ Phase of Tungsten Compared to the Original α Phase

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Tungsten holds immense promise as a plasma-facing material in fusion reactors. However, helium bubble formation and the resulting structural changes raise concerns about its long-term performance. To address these issues, it is crucial to have a detailed understanding of the changes that occur within tungsten during the fusion process. A significant change is the helium pressure-induced phase transformation in tungsten from its body-centered cubic α phase to the face-centered cubic γ phase. This study investigates helium clustering behavior within both the α and γ phases of tungsten using density functional theory. Our calculations suggest that helium clustering is less favorable in the transformed γ phase compared to the α phase, indicating that the γ phase is more resistant to helium-induced degradation.

Keywords: ab initio calculation; deformation structure; defects

2D Hybrid Materials for Brain-inspired Computing and Associative Learning

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Cost-effective solution-processed memristor devices present considerable promise for enhancing synaptic applications, providing scalable, affordable, and efficient options for future neuromorphic systems. These devices mimic the behavior of biological synapses through their gradual and continuous resistance changes, making them highly attractive for neuromorphic computing and artificial neural networks. Herein, a hybrid materials-based active layer is introduced to discuss the conductive filament-assisted resistive switching in a solution-processed active layer comprising thermally exfoliated graphitic carbon nitride (g-C_3N_4 or CN) nanosheets embedded with silver nanoparticles (Ag NPs). The fabricated devices exhibit reliable bipolar memory characteristics with a low operating voltage, effectively emulating synaptic plasticity dependent on the frequency and amplitude of the voltage pulses. The threshold switching is attributed to the formation of conduction filaments (CFs) of silver ions (Ag^+). The experimental results showcase the potential for applications in associative learning and Morse code detection.

Interplay of Dipolar Interactions and Magnetic Anisotropy in Rare Earth substitute Ferrites: A Path to Improved Self-Heating for Magnetic Hyperthermia Applications

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Hyperthermia is one of the cancer therapy which is considered to be an artificial way of increasing the body tissue temperature by delivering heat obtained from external sources to remotely destroy cancerous cells or prevent their further growth. The relevant physics in Ferrite-Based Magnetic nanoparticles and their response to the heat generation validates the efficacy for the approach. In single-domain superparamagnetic nanoparticles the magnetic anisotropy play an important role in modulating the energy barrier and hence heat dissipation by the magnetic nanoparticles. However, the role of magnetic anisotropy in controlling self-heating efficiency is a topic of debate. The debate surrounding the role of magnetic anisotropy in self-heating efficiency stems from the complex interplay of various factors involved in the heat generation process. Thus, understanding the physics of magnetic nanoparticles and controlling their magnetic properties represent hot topics not only for fundamental studies but also for technological applications. In this talk, I will first introduce the basic mechanism behind the magnetic hyperthermia and will discuss the effect of magnetic anisotropy to control self heating response in reference to the recent finding of rare earth substitute ferrite based magnetic nanoparticles. This lecture will combine insights into fundamental physics of magnetic nanostructures along with recent research advances in their application to magnetic hyperthermia.

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Heavy Transmission Metal and Metal-oxide: Hard Coating to Quantum Dots

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It has been realized that the heavy metals: molybdenum (Mo), tungsten (W), and rhodium (Rh) are preferred materials for the fabrication of plasma-facing and the optical diagnostics components of fusion reactors such as First Mirrors (FMs). All these heavy metals have high reflectivity, high electrical conductivity, high melting temperature and mechanical strength, good metal barrier performance, fine patternability, etc. The thin films of these metals are potential alternatives to the bulk FMs. Therefore, there is a need to investigate the physical properties of these thin films.

Apart from this FM application, Quantum Dots (QDs) of heavy metal oxide such as MoO_3 have potential application in Volatile Organic Compound (VOC) gas sensors. Generally, the synthesis of QDs is broadly classified into two approaches: top-down and bottom-up. The top-down approach mainly depends on weakening the van der Waals interactions between adjacent layers and breaking the strong covalent bonds of the material. Top-down approaches, such as laser ablation, e-beam lithography, can be used to reduce the particle size. Unfortunately, such methods are weakly feasible for high-yield QDs synthesis. On the other hand, bottom-up approaches need insulating ligand coating, which affects the electrical transport properties of the material. Several difficulties persisted in the existing synthesis procedure of Transition Metal Oxide QDs as per the present literature survey. It depicts that there is a need for an alternative approach to synthesize QDs without any incongruities.

In this work, key features of Mo, and W thin film deposition by pulsed laser deposition technique; and highly stable and water-soluble MoO_3 QDs without any surfactants synthesized by a hybrid method will be presented. The growth mechanism of QDs in different crystalline phases was investigated as a function of several growth parameters. The mechanism behind the controlled size of the QDs deeply rooted in the acoustic cavitation phenomenon. The dispersion parameters viz: oscillator energy, dispersion energy, transition moments, static refractive index, oscillator strength, and oscillator wavelength were also estimated via Wemple-DiDomenico (WDD) single oscillator model.

Keywords: MoO_3, Quantum Dots, band-gap

Oral Presentation

White Light Emitting Spin Active Excitonic States in Mn Doped CdSe Layered Nanosheets

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The two dimensional semiconductor layered nanosheets with enhanced coulomb interaction between the in-plane-confined electron and hole leading to strongly bound exciton are an active domain of research for realization of the excitonic circuit [1] and solid state laser [2]. The tuning of exciton dynamics through spin-orbit interaction [3] provides a superior controlling channel to achieve smart photonic devices. Insertion of spin degrees of freedom in the LNSs by doping of transition metal, activates a long range magnetic ordering suitable for spin-photonics and carrier-induced magnetism applications. As an effort towards improving the spin polarized excitonic properties, the manganese doped cadmium selenide layered nanosheets (LNSs) have been synthesized and characterized by transmission electron microscopy, Raman spectroscopy and electron paramagnetic resonance spectroscopic characterizations. The microscopic and spectroscopic investigations revealed a well-defined layered nanosheets exhibiting novel physical and optical properties. The spin dominated optical properties in manganese doped cadmium selenide ultra-thin (thickness ~1.5 nm) layered nanosheets are demonstrated. Our studies reveal the presence of magnetic ordering up to 48 K and co-existence of the multivalency Mn based local structures corroborated to the x-ray absorption near-edge structure and Raman scattering measurements. The room temperature based optical absorption and photoluminescence (PL) measurements affirm the emissions corresponding the band edge and dopant level mediated transitions to white light emission. The temperature dependent PL analysis confirms the tuning of the binding energy of exciton-Mn hybridized state to 80 meV due to the confinement mediated intermixing of wave functions [4]. The time resolved PL decay measurements accomplish the excitonic magnetic polaron states (life time ~ 14 ns). The circularly polarized magneto-PL studies at 2 K corroborated a giant Zeeman splitting with effective Lande-g as high as 172. This opens up the possible applications of the LNSs in large scale spin-active continuum photonic source.

Keywords: Layered Nanosheets, spin polarized exciton, photoluminescence, Zeeman splitting

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Non-invasive Nitric Oxide Sensing in Body Fluids for Biomedical Application

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Nitric oxide (NO) is one of most important cellular signaling molecules responsible for blood pressure regulation, vasodilation, neurotransmission, immune response and several physiological process. Any deviation of NO concentration in body fluids causes deadly diseases like Parkinson's disease, fibrosis, hypertension, rheumatoid arthritis etc. Noninvasive detection of NO in our body fluids is very much attractive for early prediction of our health condition. Here, we report the fabrication of nanomaterial based electrochemical sensors which selectively detect NO in fluids like human saliva and artificial tears. Pt decorated titanium dioxide (TiO_2) nanoparticles (Pt-TiO_2 NPs) were studied for NO sensing in human saliva. Fig. 1(a) shows typical transmission electron micrograph (TEM) of Pt-TiO_2 NPs deposited on carbon based screen printed electrode. The amperometric i-t response of the sensing electrode with raw saliva and NO added saliva is shown in Fig.1(b). The digital photograph of the electrode is presented at the inset of Fig.1(b). The amperometric i–t response clearly demonstrates NO detection in human saliva. The sensor demonstrated high sensitivity (~7.8 **$\mu A\ mM^{-1}cm^{-2}$)** in wide linear detection range (10 *n*M-28 mM) **and demonstrated ultra-low detection limit (**~2.4 nM**).**

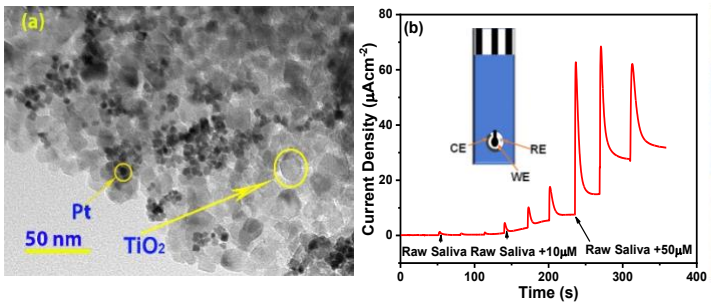

Fig. 1: (a) TEM micrograph of Pt-TiO_2 NPs and (b) NO sensing results with commercially available carbon based screen printed electrodes.

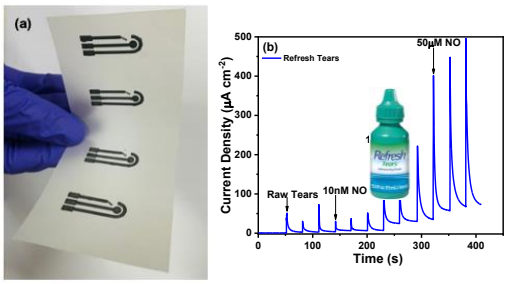

Fig. 2: (a) Photograph of paper based electrodes. (b) amperometric i-t response of Au-CC working electrode with raw and NO added artificial tears.

A paper based Au nanoparticle deposited carbon cloth sensing electrode (Au-CC) was studied for electrochemical NO detection in artificial tears. Working electrode, reference electrode and counter electrodes were fabricated by painting carbon ink on paper substrates. Fig. 2(a) shows carbon ink-based electrodes painted on paper substrate. The amperometric i-t study with artificial tears (Fig. 2b) exhibiting excellent NO detection using a low cost paper based electrode. Such electrode demonstrated sensitivity of 0.42 $\mu A\ \mu M^{-1}$ in the linear range 10nM to 1.4 mM. The detection limit of the NO sensor was achieved 2.3 nM. Both the above sensing electrodes are highly stable, reproducible and selective towards NO among various interfering agents present in saliva and tears. This study demonstrated the potential used of paper based electrochemical NO sensors for biomedical applications.

Keywords: NO sensor, Pt-TiO_2 NPs, Au NPs, Carbon Clot

Nanostructure based Triboelectric Nanogenerators for Self-powered Sensors

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In today's world, the Internet of Things (IoT) has revolutionized the society though the modernization of education, healthcare, transport, security, robotics, agriculture. The exploitation of IoT based electronic gadgets in usual activities have transformed human life. However, the extensive deployment of these devices may worsen the worldwide energy crisis. Most of these gadgets are constituted of two important components; the sensor and the power source. Thus, development self-powered gadgets can be a possible route to overcome this situation. Recently triboelectric nanogenerators (TENG) have evolved as tiny power sources for flexible and wearable gadgets. Again, the dependence of TENG output on the environmental conditions are favorable for self-powered sensing applications. From device point of view, the exploitation of nanostructured materials in TENG is advantageous to achieve flexible power sources and sensors. Nanostructures of ZnO with diverse morphology is a promising material for TENG application. The ZnO nanorods grown on cotton cloth is promising sweat sensing application [1]. The sweat sensing characteristics of ZnO-based TENG on a textile platform can be explained through the change in conductivity of ZnO and rise in generated output during sweat-nanorod interaction. Again, the influence of temperature on the output of ZnO based TENG is promising for temperature sensing application [2]. The evolution of nanowall like structure offers more contact area and hence generates higher TENG output. The deployment of such TENG patches on finger can generate diverse electrical signals and is beneficial for tactile and gesture sensing application [3]. Further investigation of TENG output in diverse humidity and gaseous conditions is attractive for monitoring fruit freshness in agricultural sector. Thus optimization of TENG active material and device structure may pave the path for achieving self-powered gadgets applicable in wide spectrum of the society.

Keywords: Triboelectricity; Energy harvesting; Sensor; Flexible electronics

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DFT study of Chlorophyll as a $OH^{\bullet}$ radical scavenger

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Chlorophyll is a green pigment present in plants and fruits. Chlorophyll is considered to have antioxidants properties and is used as medicines to cure many diseases. Under oxidative stress the amounts of free radicals surpass the number of antioxidants in our body, thereby surge in the levels of oxidants occurs, which causes various diseases including aging and cancer. $OH^{\bullet}$ radicals which belongs to ROS (Reactive Oxygen Species), causes structural damage to the important biomolecules that include DNA, proteins, lipids etc in our body. Structural damage to the important biomolecules is responsible for the cause of many diseases. $OH^{\bullet}$ radicals are generated in our body by photolysis of water, Fenton reaction and Haber Weiss process. Antioxidant which are taken from outside has the ability to deplete the excess production of $OH^{\bullet}$ radicals by adopting three major radical scavenging mechanisms viz RAF, HAT and SET. In this presentation using DFT, all these mechanisms were explored to investigate the $OH^{\bullet}$ radicals scavenging abilities of chlorophyll molecule. Due to the large size of chlorophyll molecule, ONIOM calculations were performed. The carbon centred atoms of the porphyrin ring are the sites of RAF reactions, and H atoms are abstracted from the porphyrin ring as well as from the phytal chain of the chlorophyll molecule both in gaseous and aqueous phase. SET reactions are not viable in both the media.

Keywords: $OH^{\bullet}$ radical, chlorophyll, DFT, ONIOM

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Electronic Structure And Thermoelectric Properties Of Ferromagnetic Heusler Alloy CoVZrAl

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The thermoelectric (TE) materials are considered to be a promising materials for controlling global warming and achieving a sustainable environment. These TE materials can generate electricity from waste heat in environmental sources by utilizing the principle of Seebeck effect. Using first-principles electronic structure calculations, we study the formation energy, the elastic properties and the equilibrium lattice parameter, electronic and thermoelectric properties of the quaternary Heusler alloy CoVZrAl, obtained by 50% doping at the Co site of Co_2ZrAl with localized 3d electrons of V. The first-principles electronic structure calculation performed using density functional theory (DFT) reveals that CoVZrAl is a semiconductor with a small yet finite band gap in its ferromagnetic phase [1]. It shows a magnetic moment in agreement with Slater-Pauling rule and hence is a potential spin filter material. The thermoelectric properties mainly described by the Seebeck coefficient (S), electrical conductivity (σ/τ), electronic thermal conductivity (κ_e/τ), power factor (P.F) and thermoelectric figure of merit (ZT) are determined within the framework of the semi-classical Boltzmann transport theory under the relaxation time (τ) approximation. The thermoelectric figure of merit for n-type CoVZrAl reaches a moderate value at 800 K. The microscopics behind the high ZT are explained [2] and further avenues for improvement are suggested.

Keywords: Heusler compound, band gap, Seebeck coefficient, thermoelectric figure of merit

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Impact of Oxygen Vacancy Defects on MgO Multi-layer Systems

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We have systematically investigated the structural and electronic properties of MgO bi- and tri-layers with and without oxygen vacancies. The DFT study indicates that both layer number and stacking pattern significantly affect the electronic structure of MgO multi-layers. However, these systems undergo significant reduction in electronic energy gap in the presence of oxygen vacancies. Consequently, the optical response of these multi-layered systems highly undergoes energy red shift in comparison with the pristine form. Moreover, concentration and position of oxygen vacancy defects strongly govern the optical activity of the MgO multi-layer systems. Therefore, such approach may be fruitful to achieve suitable materials for optoelectronic applications.

Keywords: MgO bi- and tri-layers; Structural Properties; Electronic Properties; Optical Properties

Theoretical Analysis of Temporal Domain, Spatial Grids and Time Steps of Soliton Wave with Reference to Energy Loss

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In optical fiber communications, solitons facilitate the transmission of high-capacity data over long distances without frequent amplification or regeneration. Solitons are self-reinforcing solitary waves that maintain their shape and velocity during propagation, arising from a balance between nonlinearity and dispersion in a medium. In this present work, we present a study and analysis of parameters such as temporal domain, number of time steps, spatial grids, amplitude, and width of a solitary wave. Our observations shows that decreasing amplitude, spatial domain of soliton wave and increasing the width, spatial grids, and time steps result in finer graphs for minimizing energy loss. Our theoretical work is based on Python code for soliton solutions of Gross-Pitaevskii equation (GPE), a well-known equation in the context of Bose-Einstein condensates. The result shows reducing energy loss by numerical simulations often entails improving the numerical stability and accuracy of the simulation. Solitons find applications in nonlinear optics, where their interactions can generate new frequencies through phenomena such as frequency conversion and supercontinuum generation and are utilized in the fields of fiber lasers, optical microscopy, and spectroscopy, enabling the production of ultrashort pulses for precision measurements and material characterization. In short, solitons play a crucial role in modern optical communication and nonlinear optics, offering a robust and efficient means of signal transmission and manipulation with broad applications in various scientific and technological domains.

Keywords: Temporal domain, spatial grids, width of a solitary wave, time steps of Soliton wave

Thermodynamical, Structural, Electrical, Non-linear Optical and Vibrational Studies of TB10A using DFT

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This article presents physical, vibrational, nonlinear optical and thermodynamical properties study of a Schiff base liquid crystal (LC) N,N-(terephthalylidene)bis(4-decylbenzenamine) (TB10A) using density functional theory(DFT). The optimized structure of TB10A is obtained using DFT with B3LYP functional and standard basis set 6-311G (d, p). From the optimized structure thermodynamical properties, electric properties, frontier orbital, atomic polar tensor (APT), electrostatic potential surface, nonlinear optical properties, infrared spectra and Raman spectra are computed.

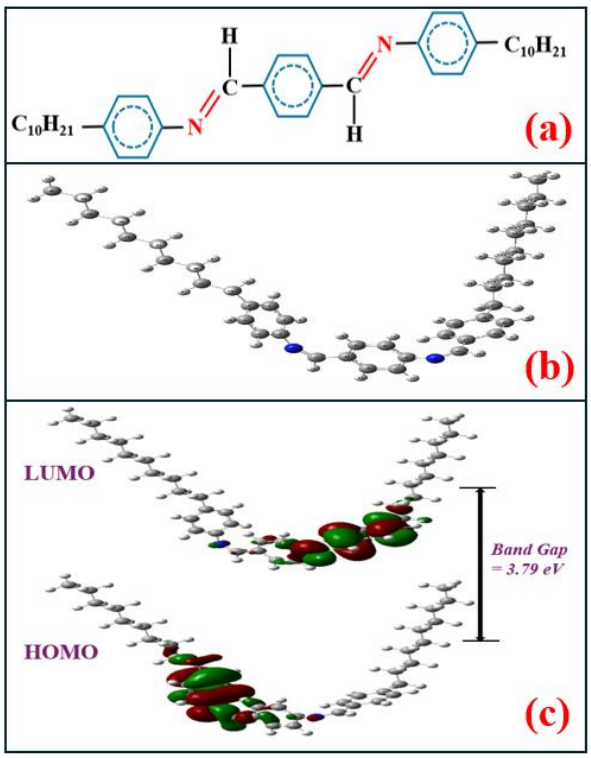

Fig. 1: TB10A (a) Structure of TB10A. (b) Optimized structure of TB10A using DFT/B3LYP 6-311G(d,p) basis set. (c)Frontier orbital analysis of TB10A using DFT

TB10A has a staggered core consists of three benzene rings connected by Schiff's base linkages, where the middle benzene ring is symmetrically substituted, and the peripheral benzene rings are unsymmetrically substituted. Thermodynamical properties such as zero-point vibrational energy (ZPVE), total thermal energy, total specific heat capacity, rotational constants and total entropy provide a better understanding of the compound. Electrostatic potential and APT gives a visual picture about the electric charge distribution in the molecule and reactive sites of the molecule in a reaction. It is found that TB10A has a lower value of HOMO-LUMO energy gaps of 3.79eV along with highly fascinating nonlinear optical properties. The NLO properties of the compound exhibit significantly higher value suggesting potential utility in NLO-based applications. The DFT calculated IR and Raman spectra shows excellent agreement with the experimentally results available in literature. IR and Raman spectra of TB10A is analysed for their vibrational modes using VEDA. This work also opens a new path for further investigations into optoelectronic applications and molecular dynamics of such compound.

Keywords: Liquid crystal, DFT, Vibrational Analysis, NLO

$WO_3.H_2O$ Engineered Polymeric MXene Membrane for Multifunctional Applications

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Multifunctional membranes have garnered continuous attention in the field of water purification due to their ability to separate oil-water mixes and break down organic contaminants found in water. Herein, a Ti_3C_2 MXene embedded polymeric membrane was synthesized employing electrospinning technique. The exposed surface of electrospun PVDF fibers had a consistent distribution of a well-defined Ti_3C_2 MXene. Later $WO_3.H_2O$ flowers like micro-structures were successfully decorated over the electrospun fibers using hydrothermal approach. The porous superhydrophilic multifunctional membrane could effectively separate oil-water mixes and degrade dye with a high degradation efficiency. The composite membrane reveals high separation fluxes (i.e., 1834-2090 $Lm^{-2}h^{-1}$) and high separation effectiveness (~99%) for a variety of oil-water mixes. Furthermore, $WO_3.H_2O$ and metallic Ti_3C_2 MXene with good facial contact have properly matched energy level alignment, which facilitates charge carrier transit and segregation. The composite membrane exhibits refreshing behaviour and outstanding recyclability. In the field of wastewater treatment, $WO_3.H_2O$ flowers-like microstructures adorned polymeric MXene membranes sound to be an excellent prospect. Additionally, this method can be expanded to create multifaceted membranes for wastewater treatment that feature other metal oxide nanostructures.

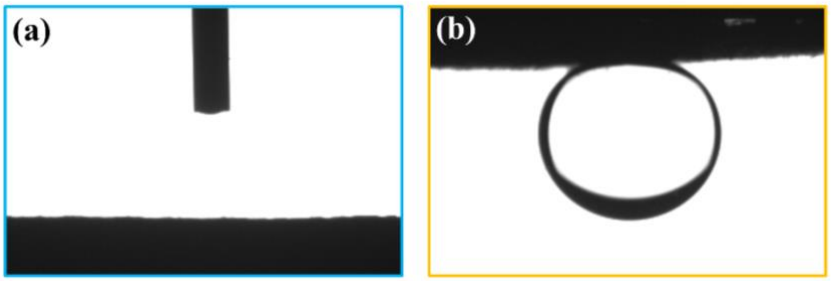

Fig. 1: (a) WCA and (b) UWOCA of Ti_3C_2/ $WO_3.H_2O$ composite membrane

Keywords: Ti_3C_2 MXene, $WO_3.H_2O$ micro-structures, oil-water separation, photocatalytic activity

Magnetostructural Transitions Induced by the Intermediate Spin State of Co in Lanthanum Cobaltite

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Lanthanum cobaltite ($LaCoO_3$) exhibits distinct characteristics in comparison to other compounds in the $LaMO_3$ (M = transition metal) series, primarily due to the emergence of additional spin-degrees of freedom. The complex interplay of various degrees of freedom, including orbital, electric, magnetic, and structural, arises from the strong correlation effects exhibited by the 3*d* electrons and their hybridization with the oxygen 2*p* orbitals. These new spin-degrees of freedom gives rise to the existence of unusual low-temperature structural transitions [1,2]. The *d* electrons of trivalent cobalt ions located at the center of CoO_6 octahedra within the $LaCoO_3$ perovskite is highly susceptible to crystal field splitting. The *d*-electron spin-states are largely influenced by the crystal field energy and Hund's coupling of Co^{3+} ions. Consequently, the electronic states of cobalt strongly influence the physical properties of the system, which can be tuned by elemental substitution at either the *A* or *B*- sites. Here, we present a systematic study on the role of Jahn-Teller (JT) distortion and its influence on the structural and magnetic properties of the $La_{1-x}Pr_xCoO_3$ (LPCO) system. In the present scenario, we have employed the sol-gel method to produce bulk and nanocrystalline forms of the perovskite LPCO with compositions ranging from 0 to 0.9. The study is primarily concerned with investigating the varied and intertwined spin states of electrons in Co^{3+} ions within LPCO. These spin states exhibit a significant correlation between the crystal and magnetic structure of the material. The structural analysis of these compounds reveals a phase crossover from the monoclinic (space group, s.g.: *I2/a*) to orthorhombic phase (s.g.: *Pbnm*) for the bulk polycrystals, while, a structural transition from the rhombohedral phase (s.g.: *R-3c*) to an orthorhombic one (s.g.: *Pnma*) is observed for the nanostructures, when $0 \leq x \leq 0.6$. Such structural transformations signify the dominant role of the JT distorted intermediate spin state $t_{2g}^5e_g^1$ ($S = 1$) of Co^{3+} cations in the investigated system (Fig.1). Thus, our study reveals that the intermediate spin-state of Co^{3+} play a crucial role in the physical properties of $LaCoO_3$ and its substituted derivatives.

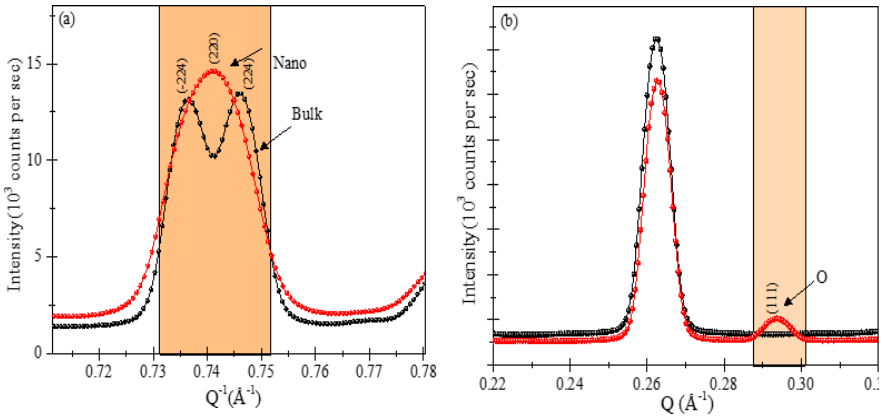

Fig. 1 (a): An enlarged view of the nano and bulk LPCO synchrotron *x*-ray diffraction patterns showing rhombohedral and monoclinic structure, respectively. (b) Bulk polycrystalline LPCO exhibiting monoclinic to orthorhombic structural transition which is evidenced by the appearance of a new peak at 0.29 $Å^{-1}$.

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Investigation of Phonon Spectral Function of Holstein Polaron within Ward Identity Preserving Approach

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We investigate the impact of electron-phonon coupling induced many-body effects of phonon spectral function of the Holstein polaron. Our investigation is based on the Ward identity preserving approach [1] where many-body effects are incorporated in terms of electron self-energy and vertex correction. In this approach the net many-body correction vanishes for **q**=0 mode due to exact cancellation between the contribution from electron self-energy and vertex correction as the consequence of the charge preserving Ward identity.

Keywords: Holstein polaron; self-energy; vertex correction; Ward identity

References:

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Preparation and optimization of phosphate loaded CMC/ZnO/Ni cross-linked nanocomposite hydrogel beads for agricultural application

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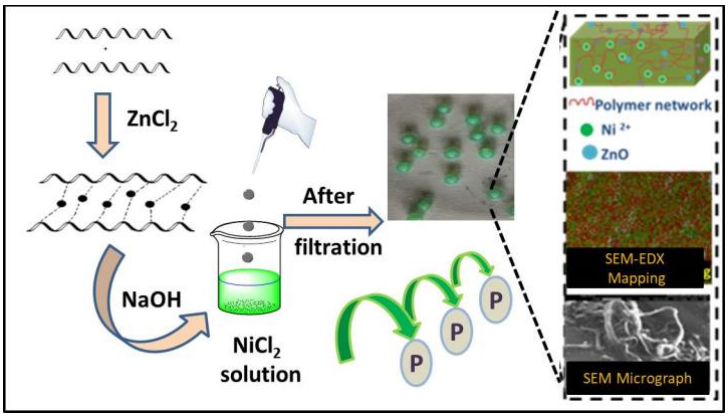

Fig. 1: Schematic representation of propose work

The present study decerns a novel synthetic protocol for the preparation of nickel-zinc oxide (plant micronutrients) crosslinked carboxy methyl cellulose (CMC) nanocomposite hydrogel bead loaded with phosphorus (P) as a slow release phosphatic fertilizer. A 1:0.15 ratio of 4% CMC solution and zinc chloride ($ZnCl_2$) was found to be optimum for the formation of stable spherical hydrogel beads when added dropwise in nickel chloride ($NiCl_2$) solution (3g in 10mL). For the phosphate loading and release study, CMC (2g) was introduced onto disodium hydrogen phosphate solution (4%) during the synthesis process keeping the rest of the procedure same. The prepared composite beads having P, Ni and Zn were thoroughly characterized using fourier-transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), scanning electron microscopy (SEM), and SEM-energy dispersive X-Ray (SEM-EDX) mapping analysis. The prepared optimized composite bead was also found to be a potential slow-release phosphatic additive for agricultural delivery within a time span of 21 days. The degradability of the composite hydrogel beads resembling different soil pH was also evaluated. The findings coincide with other studies and proved its sustainable controlled nutrient release behavior as a unique nutrient source for agricultural applications.

Keywords: CMC, Biodegradable, Hydrogel, Slow-release fertilizer

$CsPbBr_3$/PVDF-HFP and ZnO Nanorods based Tribo-Piezoelectric Hybrid Nanogenerators for Self-powered Photodetection Application

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The development of Internet of Things (IoT) based sensors has increased the demand for external power sources. One of the techniques to develop self-powered sensors is the use of a Triboelectric Nanogenerator (TENG), which operates on the principle of contact-electrification and charge induction. TENG harvests mechanical energy from the surrounding environment or biomechanical movements, aiming to reduce the excessive use of conventional power sources and overcome the limitations of old battery techniques. Here we report a single electrode tribo-piezoelectric hybrid nanogenerators (STPHNG) based on CsPbBr3/PVDF-HFP and ZnO nanorods for UV to visible light phototdetection. We studied the performance of the STPHNG under dark and light illumination conditions. When exposed to UV or visible light, the STPHNG showed a decrease in the generated output due to the screening effect of tribo-charges. Our STPHNG demonstrated a responsivity of approximately 3.59x104 V/W for UV and approximately 6.13x104 V/W for visible light. Additionally, we attached a prototype sensor to human fingers for real-time photodetection during biomechanical movements under dark and light illumination conditions. Furthermore, we successfully demonstrated wireless data transmission using a microcontroller unit.

Keywords: contact-electrification; nanogenerators; photodetection; perovskite

Biochar from *Musa cheesmanii* Waste: A Comprehensive Approach for the Removal of Fe(II) from Aqueous Environments

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The utilization of biomass feedstock material presents multiple advantages in the production of activated carbon based on its cost-effectiveness, accessibility, distinct physical and chemical characteristics. This work reports the conversion of biomass (*Musa cheesmanii)* into activated biochar *via* H_3PO_4 as an adsorbent for decontamination of Fe(II) from aqueous solution. The Taguchi experimental design (L_{16} orthogonal array) was used to complement the batch adsorption and to decrease the number of experimental runs. L_{16} orthogonal array based on the signal to noise ratio (Larger is better) suggest the maximum sorption uptake was achieved at pH 7, carbon dose of 0.25 g, and agitation speed of 200 rpm. The Langmuir isotherm fit the experimental equilibrium data of Fe(II) adsorption onto the adsorbent with maximum adsorption capacity at 7.6 mg g^{-1}. Kinetic experimental data for the adsorbents was best described by the pseudo-second-order equation indicating a chemical sorption process.

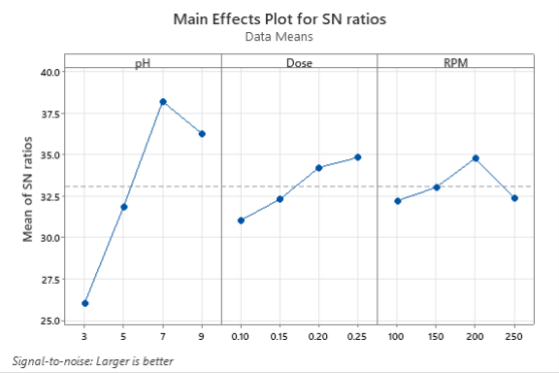

Fig. 2: S/N ratio for the observed L16 orthogonal array

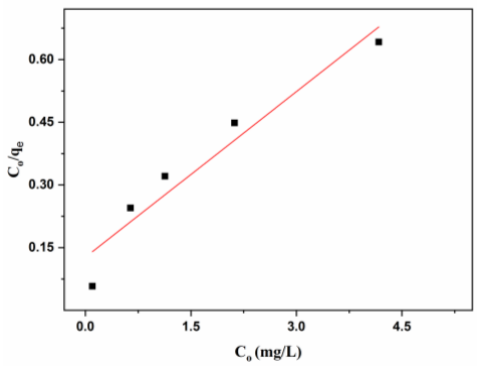

Fig. 2: Langmuir isotherm model indication better fitting for the data

Keywords: Biochar, Cost-effective, Taguchi, Isotherm

Acetone Gas Sensing using Molybdenum Disulfide Films Fabricated by Vapor Plasma Mixing Technique

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Acetone (CH_3COCH_3), a hazardous volatile organic compound (VOC), is commonly employed in numerous scientific and domestic applications. A prolonged exposure to high levels of acetone can lead to several adverse health effects, including respiratory irritation, dizziness and headaches. The development of advanced acetone sensing equipment is crucial for safeguarding workplace safety and mitigating the adverse health effects associated with acetone exposure. Additionally, acetone detection plays a vital role in the diagnosis of diabetes. Human breath contains a complex mixture of VOCs, including acetone. Elevated levels of acetone in exhaled breath is a key indicator of diabetes. Early diagnosis and treatment of the disease are possible through accurate measurement of acetone levels. Consequently, this study investigates the use of molybdenum disulphide (MoS_2) thin films as a potential material for acetone sensor fabrication. These films were fabricated using a novel deposition technique involving the simultaneous sputtering of molybdenum plasma and thermal evaporation of sulphur vapor in a high-vacuum environment. The resulting films were characterized through Raman spectroscopy and surface morphology analysis. To evaluate the sensing performance, the electrical response of the MoS_2 films was measured in the presence of air and acetone at varying operating temperatures. The results indicate a significant enhancement in sensitivity with increasing temperature.

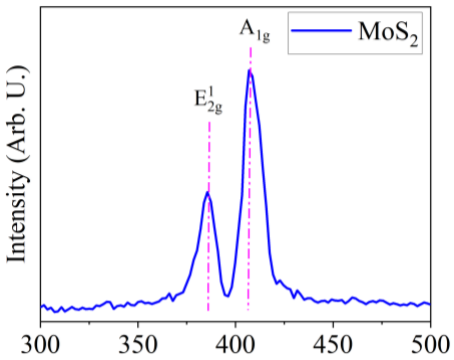

Fig. 1: Raman Spectra of the as-deposited films

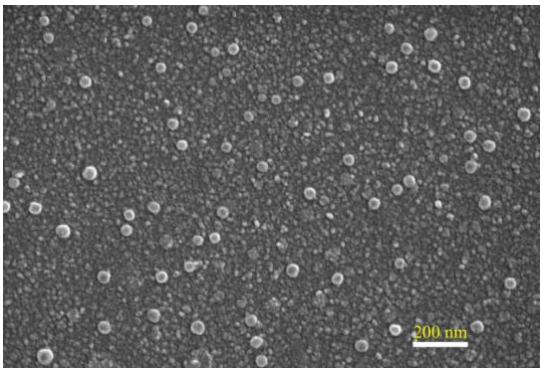

Fig. 2: SEM image of the as-deposited films

Keywords: MoS_2 thin films, Raman Spectroscopy, Acetone Gas Sensing

Noticeable Improvement in the Electrical Conductivity of Zr-based UiO-66 Metal Organic Framework (MOF) with Incorporation of Ag_2O Nanoparticles

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Metal-organic frameworks (MOFs) are versatile materials with applications ranging from gas storage to catalysis, but their inherent low electrical conductivity has historically limited their utility in electrochemical applications, such as batteries, supercapacitors and sensors [1]. To overcome this limitation, researchers have explored strategies like incorporating redox-active organic linkers, mixed-valence metal centers, and conjugated linkers into the MOF structures. These modifications enhance conductivity by promoting charge transfer pathways, facilitating electron delocalization, and introducing additional charge carriers within the material [2]. These methods have improved the desired characteristics considerably, but compared to conventional MOFs, there are far less of these building blocks [3]. In response, this study adopts a different approach by employing post-synthetic modification to introduce metal oxide nanoparticles (NPs) into MOF structures. Specifically, we focus on incorporating silver oxide nanoparticles (Ag_2O) into the Zr-based MOF UiO-66. To achieve this, Ag_2O NP has been loaded into UiO-66 MOF using two distinct methods for post-synthetic modification. One uses a natural reducing agent, while the other uses a conventional one, and the yield products are denoted as Ag_2O@UiO-66-S1 and Ag_2O@UiO-66-S2. In the case of Ag_2O@UiO-66-S1, the NPs reside within the microcavities of UiO-66, but in Ag_2O@UiO-66-S2, the particles are generally present on the surfaces of the UiO-66 particles. The electrical properties of these modified UiO-66 samples were investigated using the two-probe *I-V* method. Remarkably, the results demonstrated a significant increase in electrical conductivity, with enhancements of 100-fold observed in the modified samples compared to its UiO-66 pristine counterpart. Further analysis revealed that the charge transport mechanism was predominantly governed by thermionic emission of charge carriers. Importantly, despite the improvement in electrical properties, the materials retained their microporous feature, suggesting their potential in electrochemical applications including electrode preparation and sensor design consideration.

Keywords: UiO-66, MOF, Ag_2O NP, electrical properties

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Formation of anomalous Andreev bound states in Ising superconductor |Half-metal| Ising superconductor

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In this work, we have studied the formation of Andreev levels and supercurrent in a clean Ising superconductor (ISC)/half metal (HM)/Ising superconductor (ISC) Josephson junction (JJ) with spin-active interfaces using Bogoliubov-de Gennes formalism. The impact of spin-mixing, spin flipping and spin-orbit coupling (SOC) on the Andreev bound states (ABS) spectra and current phase relationship (CPR) have been explored for both transparent and opaque barrier limits. Our result indicates an additional splitting of the Andreev levels due to the combined effect of spin active barrier moment and SOC of the ISC. Thus, a possible $0-\pi$ transition for different barrier magnetic moments can also be achieved. By adjusting the spin mismatch angle and the strength of the barrier magnetic moment different φ – junctions can be realized. Additionally, by adjusting the control parameters a $0-\pi$ transition can also be achieved for JJs with stronger SOC than the chemical potential of the ISC. Moreover, anomalous Andreev levels were observed for different HM lengths which indicates its significant role in tuning the φ - phase Josephson junction.

Keywords: Andreev Bound States, Ising Superconductor

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Development of a New Generation Glassy Electrolyte to Study their Mixed Alkali Effect with Enhanced Characteristic Properties

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A new glassy system Na_2O-Li_2O-ZnO-$PbCl_2$ has been developed with $PbCl_2$ as network former and ZnO as stabilizer in order to study the mixed alkali effect of the system that acts as electrolyte for a battery. The XRD pattern of the system were analysed to study the microstructural properties of the system. Their various nanophases were obtained from the XRD analysis. The AC and DC conductivities of the system were studied as a function of frequency. The parameters such as hopping frequencies, low frequency conductivity, frequency exponents were also analyzed using Almond-West formalisms. The system under study showed fluctuation when their DC conductivity was plotted against the relative compositions Na/(Na+Li) at a particular temperature. The plot showed minima which establishes the mixed alkali nature of the system at a particular relative composition. The DC conductivity of the system were compared with other's works. Although the graph shows fluctuating nature it gives better conductivity in comparison to the earlier works. Apart from the conductivity the system seems to be stable within a certain relative composition range. The corresponding hopping frequency is plotted against the relative composition. This too shows similar nature as that of DC conductivity. This is also compared with other's work. The corresponding energies show maxima at almost the same compositions which are in accordance with the results. The power exponent were plotted against the relative composition which shows lower values (<1) giving the proof of presence of mixed alkali effect. Here the conduction was fully contributed by the movement of alkali ions unlike fluoride-glasses. The study from various graphs also reveals the thermally activated nature of the sample. The relaxation time τ and the stretched co-efficient β were also analysed to study the dielectric properties of the system. It was found that the overall contribution towards the conduction mechanism was from the alkali part and not from the negatively charged polarons or electrons. The mixed alkali effect overruled the contribution from anion by the positively charged cations which makes the present system suitable candidate for battery electrolytes and also for academic interest.

Permittivity Detection of Materials using Microwave Sensor

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The rapid advancement of the biomedical, food and engineering sectors increases the demand of materials characterization for their proper incorporation in the intended application. Over the years, the sensitivity of planar sensors has been significantly increased to monitor the minute variations in complex permittivity among different material samples. The use of microwave-based sensor provides higher sensitivity and resolution, therefore increasing the accuracy of measurement. The aim of this work is to determine the permittivity of dielectric materials using microwave-based sensor. The sensor is designed using High Frequency Structure Simulator (HFSS) on low cost and easily accessible FR4 substrate and is modelled to resonate at a frequency of 2.4 GHz. The extraction of the permittivity of unknown materials is then carried out using curve fitting technique involving the scattering parameters. Further, a comparison with some of the recent works based on performance parameters have been included to validate the performance of the sensor.

Keywords: Dielectric; Microwave; Sensor

Design, Synthesis and Evaluation of Potential Antibacterial and Antioxidant Properties of Ester Terminated p-substituted Aniline based Dendritic Core

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The emergence of multi-drug-resistant bacteria poses a significant threat to both public health and economy. This urgent challenge has propelled the rising trends in research aimed at developing potent antibacterial compounds. As a result, there is growing emphasis on the discovery of novel antibacterial compounds which can effectively combat this crisis. Among these, dendrimers, a unique class of polymers, have been explored as antimicrobial agents, due to their exceptional properties. Dendrimers are characterized by their regularly branched, highly symmetrical, three-dimensional structure. The dendritic structure comprises of the core, the interior branching units and the peripheral surface groups and are capable of encapsulating guest molecules. Additionally, the surface groups can be functionalized with suitable moieties for tailoring its application prospects.

In this study, we report the microwave-assisted synthesis of a series of p-substituted aniline based diadducts as dendritic core, which were characterized by Mass spectrometry, FTIR and NMR spectroscopy. The antibacterial properties of the compounds were investigated against Gram-positive bacterial species, namely, *Pseudomonas aeruginosa* and *Escherichia coli* and Gram-negative bacteria, *Staphylococcus aureus*, which revealed significant bactericidal activity at varying concentrations of the compounds, at different time intervals. The possible antioxidant property was studied using the DPPH free radical scavenging assay and the antioxidant activity of the compounds was quantified as per the IC50 values, which showed promising results, particularly in case of PAEs3. The molecules synthesised can be potential contenders for development of new drug molecules.

Keywords: antibacterial; antioxidant; dendritic core; drug resistance

Enhanced Hybridization Induced Robust Ferromagnetism in Quaternary Heusler Alloy CoIrTiAl

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The structural, electronic and magnetic properties of CoIrTiAl Heusler alloy are investigated using first -principles density functional theory. In L_{21} crystal symmetry, the equilibrium lattice constant and Bulk modulus are reported. From band structure and density of states, it is clear that CoIrTiAl exhibits half-metallic behavior having a band gap 0.5882 eV in minority spin channel. The ferromagnetic state is found to be magnetic ground state and it shows total magnetic moment 1 μ_B/ f.u. in accordance with the Slater-Pauling rule. The unpaired electron of e_u state of majority spin channel derived from Co-3d and Ir-5d electron is the main source of magnetic moment as in CoIrZrAl [1]. A 50 % doping at Co-site of Co2TiAl with Ir atom increases mean-field theory estimated Curie temperature (T_C) from 120 K [2] to much much above room temperature. This enhanced T_C makes CoIrTiAl suitable for spin injection. The charge density distribution firmly establishes that the increased hybridization between the transition metal 'd' electrons due to the presence of 5d electrons is responsible for the robust ferromagnetism in CoIrTiAl as in CoIrZrAl [1].

Keywords: DFT**,** Half-metal, Curie Temperature, Heusler alloy

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Effect of Growth Temperature on the Structural and Optical Properties of Lead (Pb) Free Cesium Copper Bromide based Perovskite Thin Films

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In the present work cesium copper bromide perovskite thin films were directly fabricated by using unique reactive vapour-plasma route. A systematic investigation was also undertaken to explore the dependence of the growth temperature of the thin films on their crystalline and optical properties. The crystalline nature of the films was confirmed from X-ray diffraction (XRD) patterns. The XRD characterization confirms the presence of two phases viz: $CsCu_2Br_3$ and Cs_2CuBr_4 in all the deposited films. The formation of nanocrystallite was confirmed by three methods viz. Scherrer's method, Uniform deformation model (UDM) and Size-Strain Plot (SSP). The nature of strain present in the films was also investigated as a function of substrate temperature. The surface morphology was investigated by scanning electron microscope (SEM) and elemental confirmation was done by energy dispersive X-ray (EDX) spectroscopy. The optical properties of the films were studied by UV-Visible spectroscopy and band gaps were estimated by using absorption spectra fitting (ASF) method. It confirms the presence of dual band gaps on the films growth at high temperature.

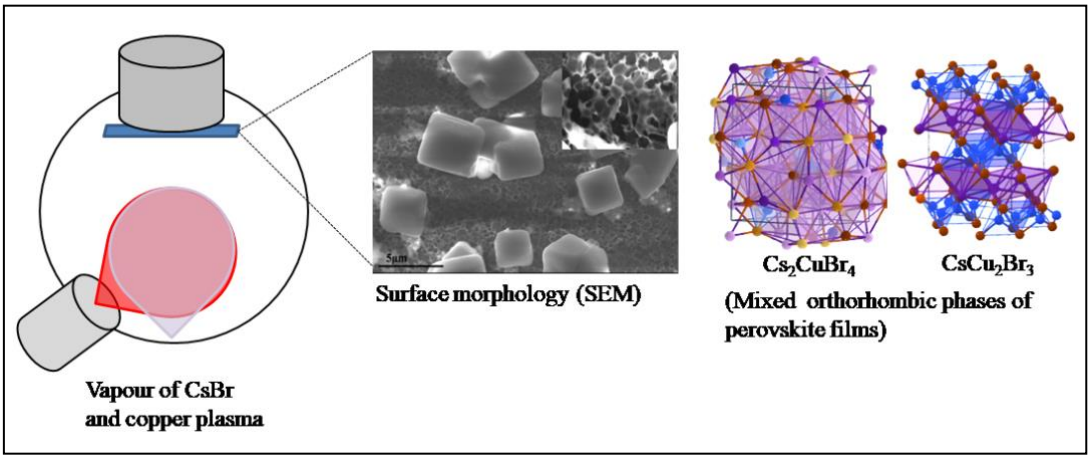

Fig. 1: Graphical abstract of present work.

Keywords: reactive vapour-plasma, thin films, RF magnetron sputtering, thermal evaporation

Effect of Doping on Superconductivity & Chemical Potential on hole-doped Iron Pnictide Superconductors

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The discovery of iron-based superconductors represented a pivotal advancement in superconductivity research, having critical temperature up to 55 K [1]. Unlike cuprates, the parent compound of these materials is as a spin density wave metal, exhibiting antiferromagnetism in its most fundamental state. The introduction of impurities disrupts this antiferromagnetic order and facilitates the emergence of superconductivity. In this study, we employ a mean-field Hamiltonian model [2] to investigate the influence of doping on spin density wave, superconductivity and chemical potential in hole-doped iron pnictide superconductors. The Hamiltonian is analyzed through the equations of motion for Zubarev-type single-electron Green's functions [3]. We derive the correlation function based on quasi-particle energies and solve for the superconducting (SC), spin density wave (SDW) order parameters and chemical potential self-consistently. Our analysis focuses on the variations in the SC gap and critical temperature across different doping levels. At zero doping, superconductivity is absent due to the presence of SDW. As doping is gradually increased, superconductivity begins to manifest at minimal doping concentrations. Further increases in doping lead to an enhancement of both the SC gap and the SC critical temperature. However, with continued doping, a gradual decline in the SC critical temperature is observed. The resulting phase diagram correlating SC critical temperature with the doping parameter aligns well with experimental observations [4]. Additionally, we study the effect of doping on chemical potential.

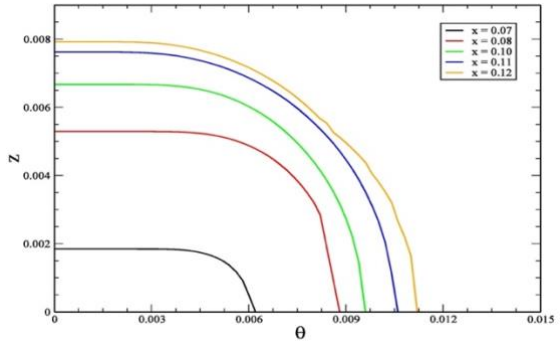

Fig. 1: Variation of SC gap & Critical temperature for different values of hole concentration.

Keywords: Superconductivity, Spin density wave, Green's function, Hole doping

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Enhanced Sunlight-Assisted Wastewater Treatment via SnO_2-Coated Jute Fibers

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In this study, we introduce a novel fabrication method for a sunlight-responsive photocatalyst designed for wastewater treatment. A biocompatible photocatalyst, "SnO_2-coated jute fiber," is synthesized using a simple, cost-effective sol-gel process followed by a hydrothermal method. The structural and optical properties of this composite photocatalyst are thoroughly investigated and compared with those of pure SnO_2. The photocatalytic performance is evaluated by degrading methyl orange, used as a model pollutant, under natural sunlight exposure. Results demonstrate that the SnO_2-coated jute fiber exhibits significantly enhanced photocatalytic activity compared to pure SnO_2. Moreover, recyclability tests reveal that the photocatalyst remains stable and effective, successfully degrading methyl orange over more than two cycles. This work highlights the potential of this biocompatible photocatalyst for sustainable wastewater treatment and its ability to address water pollution challenges.

Keywords: SnO_2, Jute fiber, Photocatalysis, Sunlight-Assisted

Strain Induced Thermoelectric Behaviour of XCaB (X = Li, Na, K) Half-Heusler alloys

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Half-Heusler (HH) alloys have been extensively explored for their promising properties, particularly in thermoelectrics, offering potential solutions to the energy crisis. The efficiency of a thermoelectric material is characterised by high Figure of merit (*ZT*) and thus improving *ZT* has been a challenging task. Strain engineering is regarded as one of the effective ways to attain a better thermoelectric performance [1,2]. In the present work, we have examined the impact of isotropic strain (up to ±10%) on electronic and thermoelectric properties of XCaB (X = Li, Na, K) HH alloys based on DFT method. The calculations are performed using Quantum ESPRESSO package and BoltzTrap code. The study shows ferromagnetic ground state (2.00 μ_B/unit cell) of α-XCaB in both strained and unstrained conditions. Compressive strain leads to increment in ductility for all compounds. The alloys are mostly half-metallic with few becoming nearly half-metallic under some strain conditions. Modification of electronic band structure results in variation of power factor ($S^2\sigma$) and electronic thermal conductivity (κ_{el}). For the half-metallic pristine XCaB (X = Li, Na, K) alloys, ZT_{el} values are 0.92, 0.96 and 0.99, respectively at 200K. It is found that the alloys exhibit high *S* and $S^2\sigma$ values for hole-type doping. Lattice thermal conductivity (κ_l) turns out to be lower for more ductile materials. The computed total *ZT* values (ZT_{tot}) including both κ_{el} and κ_l, are 0.56(LiCaB), 0.52(NaCaB) and 0.51(KCaB) at 800K. The ZT_{tot} at higher compressive strain range, experiences a notable enhancement to ~ 0.75 for LiCaB and a minor improvement to ~ 0.67 for KCaB. While in case of NaCaB, ZT_{tot} remains almost constant with the unstrained form. Thus, LiCaB appears as better thermoelectric material among the considered HH compounds.

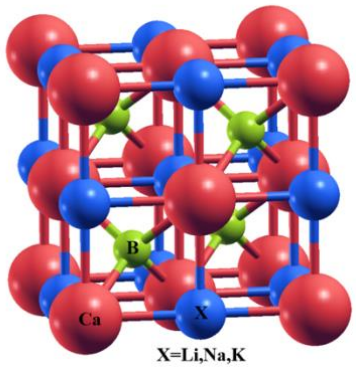

Fig. 1: Crystal structure of XCaB (X=Li, Na, K) Half-Heusler alloy

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Post Synthetic Modification of Stable UiO-66-NH_2 Metal Organic Framework as an Effective Fluorescent Probe for the Sensing of Fe^{3+} in Aqueous Medium

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Ferric metal ions (Fe^{3+}) present various environmental and biological challenges. Although they are crucial for physiological functions and enzymatic processes, either excess or deficiency can lead to health problems such as anemia, cardiovascular failure, diabetes, Parkinson's and Alzheimer's diseases. Detecting Fe^{3+} at trace concentrations is difficult and existing methods such as atomic absorption spectroscopy, chromatography and ICP mass spectrometry are expensive and complicated. This highlights the need for efficient sensing technologies for Fe^{3+}. Our study presents a facile post synthetic modification of a highly water stable Zirconium based UiO-66-NH_2 Metal organic frameworks (MOF) to a novel MOF fluorescent probe called UiO-66-NH_2-DHB MOF, which demonstrates high sensitivity and selectivity for Fe^{3+}, even at trace levels. Characterization of the material was performed using PXRD, FTIR, FESEM, XPS, TGA, BET techniques. The fluorescence study revealed that UiO-66-NH_2-DHB is highly sensitive and selective to Fe^{3+} detection, even in the presence of other interfering metal ions, with a significant detection limit of 2.3 µM. The results also showed a rapid fluorescence quenching, indicating that the probe can quickly and effectively detect Fe^{3+}. The UiO-66-NH_2-DHB fluorescent probe serves as a promising fluorescence sensor for Fe^{3+} detection, offering quick response along with excellent selectivity and sensitivity.

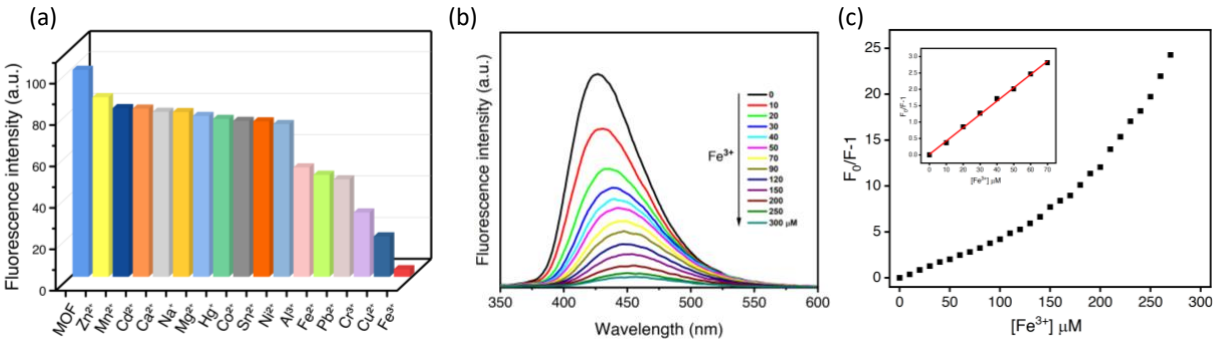

Fig.1: (a) Emission intensities of UiO-66-NH_2-DHB in an aqueous suspension upon addition of different cations (b) Emission spectra and (c) KSV curve of UiO-66-NH_2-DHB at various concentration of Fe^{3+}

Keywords: Metal organic frameworks; Fluorescence sensor, Fe^{3+} detection

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Piezo-/pyro-/photocatalysis with Ag/AZO Nanocomposite

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Semiconductors such as TiO_2, ZnO, CdSe, CuO, CdS, and ZnS have been utilized as photocatalysts for many years due to their impressive performance. Among these, the hexagonal wurtzite phase of ZnO features a non-centrosymmetric structure where the Zn ions (positively charged) are displaced relative to the O ions (negatively charged) along the *c*-axis. This lack of inversion symmetry gives rise to piezoelectric and pyroelectric effects. This work focuses on nanophase Al-doped ZnO (nano-AZO) and its nanocomposite with Ag nanoparticles (Ag NPs). The nano-AZO is prepared by the ball-mill method with a lab waste (discarded AZO sputtering targets) as the starting material and the photoreduction process is utilized to produce Ag NPs. The developed Ag/AZO nanocomposite (NC) works as a multi-functional catalyst capable of harnessing thermal, mechanical, and light energy. The piezo-photocatalysis emerges to be the most efficient with the degradation rate of aqueous methyl orange turning out to be 96.7%. The microstructure of nano-AZO is critical and a higher doping level is suitable to induce greater piezoelectric effect owing to larger microstrain and lattice distortion. The findings of piezo-photocatalysis suggest that the photothermal effect plays a significant role in enhancing catalytic performance. Additionally, the pyrocatalytic activity of Ag/AZO NC indicates a potential electrostriction effect at the Ag-AZO interface. The reactive oxygen species (ROS) play the dominant role in catalysis and a controlled scavenging of ROS is possible using biomimetic hydroxyapatite (HAp). HAp as a ROS scavenger may be utilized to regulate excessive ROS that are produced in the body due to oxidative stress.

Keywords: Ag/AZO nanocomposite, catalysis, Hydroxyapatite

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Investigation of Silica Nanoparticle Stability in Nanofluids and Its Impact on Oil Recovery in a Part of the Upper Assam Basin

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Silica nanoparticles (SiO_2 NPs) have attracted attention in Enhanced Oil Recovery (EOR) because of their unique qualities, including their large surface area, excellent thermal stability, and the ability to modify rock wettability, nanofluid viscosity, and oil-brine Interfacial Tension (IFT). Moreover, silica is naturally abundant in the sandstone reservoir rock, making the silica nanofluid flooding EOR technique environment-friendly in nature. The investigation was undertaken with the objective of evaluating the stability of silica nanoparticles in nanofluids at different concentrations and examining its effects on nanofluid viscosity, reservoir rock wettability, and oil-nanofluid IFT in a part of Upper Assam Basin. Earlier studies have shown that suspended nanoparticles can reduce the oil-nanofluid IFT and increase nanofluid viscosity, which in turn improves the recovery of oil. Also, the nanoparticles that are deposited on the rock surfaces can shift the rock wettability to a more water-wet state by forming a wedge-shaped structure, which can further enhance the recovery. A total of six nanofluids were prepared using silica nanoparticles, with concentrations ranging from 0.01 wt% to 0.50 wt% in low-salinity brine. The systematic visual inspection of the nanofluid samples shows that more silica nanoparticles remained suspended in the colloidal system it its higher concentration. Zeta potential analysis also confirms that nanofluids with higher concentrations of nanoparticles exhibited greater stability compared to those with lower concentrations. Zeta Potential up to -37.7 mV was observed in the high concentration of silica nanofluids which shows that the NPs have good stability in the colloidal system. The results of the study on IFT between crude oil and the nanofluid revealed that increasing the concentration of silica nanoparticles from 0.01% (w/w) to 0.50% (w/w) significantly reduces the IFT, decreasing it from 24.56 mN/m to 14.32 mN/m. It is also observed that the viscosity of low-salinity nanofluids increases from 1.17 cP to 1.94 cP with increasing the NP concentrations at room temperature. Furthermore, wettability alteration of the rock towards more water wetness was observed as a key silica nanofluid flooding EOR mechanism. The contact angle decreased from 48.28° to 36.21° with increasing the silica nanoparticle concentration up to 0.50% (w/w). It can be concluded that, the nanoparticles are more stable in the low salinity environment in its higher concentrations. Increasing the concentration of SiO_2 NPs in low salinity brine from 0.01% (w/w) to 0.50% (w/w) results in a decrease in both the IFT between crude oil and the nanofluid and the contact angle of the reservoir rock, while simultaneously increasing the viscosity of the nanofluid. This combination of lower IFT, enhanced water-wetness of the rock, and increased nanofluid viscosity is conducive to improved oil recovery.

Keywords: EOR; IFT; Nanoparticle; Wettability

Affordable Nanocomposite Painted Paper as Ultrasensitive SERS Substrate

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Remarkable sensitivity, selectivity, and non-destructive nature of surface-enhanced Raman spectroscopy (SERS) make it a versatile technique for the detection of trace-level analytes [1,2]. This powerful method significantly amplifies the Raman scattering signals of molecules that are either adsorbed onto or located near nanostructured metallic surfaces, offering exceptional sensitivity in molecular-level detection [1-3]. Although SERS offers notable advantages, it is accompanied by challenges such as the complexity of substrate fabrication. This work presents the development of affordable and easy-to-make paper-based SERS substrates composed of Al-Fe oxide (AFO) or cobalt ferrite (CFO) forming nanocomposite with Al-doped ZnO (AZO) and Ag nanoparticles. The AFO or CFO powders are synthesized by adopting the sol-gel method, followed by milling with nanophase AZO to produce AFO/AZO and CFO/AZO nanocomposite. The nanocomposite is applied onto a paper using a paintbrush and dried followed by the decoration of Ag nanoparticles using the DC magnetron sputtering process. Methyl orange (MO) is considered as an analyte for SERS. The AFO/AZO nanocomposite with nanostructured Ag emerges as a superior SERS substrate capable of detecting the analyte down to a very low concentration level. The paper-based Ag@AFO/AZO and Ag@CFO/AZO nanocomposites are realised as the SERS substrates, which can be easily prepared for large-scale use for the sensitive detection of analytes. The surface plasmon resonance signature is observed in the diffused reflectance spectra. Two distinct types of composites are utilized as SERS substrates: AFO/AZO, characterized by its porous structure, and CFO/AZO, which functions as a ferromagnetic material. The porous structure is confirmed by the field emission scanning electron microscopy (FESEM) images and the ferromagnetic behaviour of CFO is reflected from the vibrating sample magnetometer (VSM) data. The enhancement of Raman signals in SERS is commonly characterized by the enhancement factor (EF). The EF for the Ag@AFO/AZO nanocomposite is determined to be 10^6 at a concentration of 1 nM, and increases significantly, reaching up to 10^9 at a concentration of 1 pM.

Keywords: Affordable SERS substrates; Paper-based Ag@AFO/AZO; Ag@CFO/AZO nanocomposite; Surface plasmon resonance

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Influence of Ammonia on Chemical Bath Deposition as a Sustainable Method to Obtain $Cd_{1-x}Zn_xS$ Thin Films

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In this work, $Cd_{1-x}Zn_xS$ thin films have been deposited over soda lime glass substrate by using a simple and cost-effective Chemical Bath Deposition (CBD) method at 50^oC for a period of 30 minutes. The structural, morphological, chemical and optical properties are studied by incorporating a range of characterization techniques, including X-ray diffraction (XRD), Field Emission Scanning Electron Microscopes (FESEM), Energy Dispersive X-rays (EDX), Transmission Electron Microscopes (TEM), Fourier Transform Infrared Spectroscopy (FTIR) and UV-Visible spectrophotometers (UV-Vis). The films have been deposited at four different concentration values of ammonia which adjust the pH of the bath solution in the range from 8.5-10, which addresses in depth the structural, morphological, chemical and optical properties of the deposited films. The produced films are found to be remarkably uniform and have smooth, uncracked surfaces with distinct grain boundaries. The proposed material promises to be a potential candidate as a window layer in thin films solar cells and a good semiconductor material in optoelectronic devices.

Keywords: Thin Films; Deposition; nanostructure; TEM

Surface Wettability Features in *Bougainvillea* Flower Petals

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The wetting-dewetting behavior is a surface phenomenon dictated by both the chemical composition and roughness of a textured surface. However, many natural surfaces, including insect wings, flower petals, and leaf surfaces, have gained significant attention due to their unique yet distinctly different surface microtextures [1,2]. These surfaces can be suitably mimicked for potential deployment in next-generation coatings, packaging, microfluidic devices, and drug delivery systems [1]. Many natural surfaces, such as rice and lotus leaves, exhibit superhydrophobicity, demonstrating the '*lotus effect'* [1]. In contrast, certain flower petals display superhydrophobicity but with the '*petal effec*t,' where adhesion dominates roll-off [3,4]. In both cases, surface roughness at the micro- and nanoscale plays a crucial role [4]. For example, the coexistence of superhydrophobicity and superadhesion has recently been observed on the abaxial surface of the Indian jujube leaf [5].

In this study, the wettability features of three varieties of *Bougainvillea* flower petals are examined using a PC-interfaced contact angle meter and base tilting from 0° to 90°. To assess the adhesive properties, dynamic contact angles are measured along with contact angle hysteresis. Models are employed to explain the observed results, with surface roughness playing a significant role in the analysis. A fundamental understanding of wetting-dewetting behavior is essential for extending the scope of artificial design and biomimicry using advanced materials.

Keywords: Wettability; Roughness; lotus effect, petal effect

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A Study on the Optical Properties of Plant-based Pigment Chlorophyll and its Potential Application in the Detection of Pyrene

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Chlorophyll, an important pigment found in green plants and vegetables, plays a crucial role in the process of photosynthesis by absorbing light and converting it to chemical energy. Chlorophyll shows remarkable fluorescence properties which is widely used as a rapid, non-invasive and a suitable indicator of environmental and climatic variations. It is also an indicator of plants' photosystem and its photosynthetic activities. Due to its unique optical properties, it has found numerous applications in the field of optical biosensors, organic lasers and in the production of biohydrogen. Various anthropogenic activities such as carbon emission, release of harmful pollutants to the environment due to rapid growth of industries pose a threat to the environment. Among them, polycyclic aromatic hydrocarbons (PAH) are one of the important ones due to their carcinogenic and mutagenic effects in living organisms especially in human beings.

This study sheds light on the sensing ability of Chlorophyll and its use as a fluorescent probe in detecting Pyrene, a PAH mostly found in the areas near an oil drilling sites. They are ubiquitous and prolonged, thus posing a threat to the living organisms such as plants and animals living in that soil. The UV-Visible absorption, Photoluminescence and Fourier Transform Infrared spectroscopy were utilized in sensing Pyrene where variations in UV-Vis absorbance, PL intensities, Excited state lifetime of Chlorophyll has been considered as the sensing parameters. A limit of detection ~ 0.25 pM is observed which is significantly better than some previous reported works.

Keywords: Chlorophyll Fluorescence; Optical Sensor; PAH; Pyrene

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Surfactant-assisted Synthesis of Polypyrrole Nanoparticles in DBSA Micellar Solution: Studies of Structural, Optical, Thermal, AC Conductivity and Dielectric relaxation properties

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Conductive Polypyrrole nanoparticles (PPy NPs) have been synthesized by chemical oxidative polymerization of pyrrole (Py) monomers in a micellar solution *using* Dodecylbenzenesulfonic acid (DBSA, as anionic surfactants) with improved morphology, structural, optical, electrical and thermal properties. Ammonium persulfate (APS) as oxidant has been used to initiate the polymerization reaction and effect of DBSA micellar concentration on the formation mechanism of PPy nanoparticles has been investigated. In this micro-emulsion polymerization method, the DBSA surfactant molecules don't only provide the nano-sized micelle reactors to guide the polymerization, but also behave as dopants to facilitate the charge transfer within the polymer chains, which makes this method as a versatile, scalable and cost-effective one. Studies on morphology using scanning electron microscope (SEM) show spherical particles morphology of PPy. Structural characterization carried out by powder X-ray diffraction (XRD) technique reveals that the synthesized PPy NPs are amorphous in nature. The inter plannar (d) spacing between PPy chains has decreased with increasing the DBSA concentration. However, larger d-spacing at a higher (0.2 M) DBSA concentration has been attributed to the incorporation of large numbers of dopant counter ions in between the PPy chains. Studies on Fourier Transform Infrared (FTIR) spectroscopy have revealed chemical fingerprint of PPy NPs in all the synthesized samples. Studies of UV-vis spectroscopy have confirmed the reduction in optical band gap energy (E_g) of PPy NPs with increase in DBSA concentration. Thermo-gravimetric (TGA) studies have revealed smaller weight loss of PPy NPs upon heating in the investigated temperature range with increase in DBSA concentration. Both the frequency and temperature dependence studies on permittivity and modulus spectra DBSA doped PPy NPs have been carried out to understand the nature of polarization and relaxation mechanism charge carriers. The ac conductivity studies have shown that conductivity of PPy has increased with increasing dopant concentrations and all the samples of PPy NPs have obeyed the temperature dependent correlated barrier hopping (CBH) mechanism of charge carriers.

Keywords: Conducting Polymers; Polypyrrole Nanoparticles; dielectric relaxation; ac conductivity

Photoluminescence Behaviour of Sm^{3+} Ions in the Presence of Au Nanoparticles in silica matrix

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In the last few decades, rare earth (RE) doped materials have been a crucial area of research due to their potential application in various fields viz. phosphor, optical communication, lasers, sensors, storage devices, etc [1,2]. Nanometal-enhanced fluorescence (NMEF) is among one of the most powerful methods used to enhance the photoluminescence (PL) emission from RE ions [3,4]. The enhancement in PL is attributed to the surface plasmon resonance (SPR) effect shown by metal NPs. SPR is the collective oscillations of conduction band electrons when an electromagnetic field is incident on the metal surface.

In the present work, the effect of Au nanoparticles (Au NPs) on the PL behaviour of Sm^{3+} doped sol-gel silica matrices has been carried out. Significant enhancement in the PL intensities from the Sm^{3+} ions has been observed in the presence of Au NPs. The concentration-dependent enhancement of Sm^{3+} is explained in terms of the surface plasmon resonance shown by Au NPs.

Keywords: Rare earth, photoluminescence, surface plasmon, nanoparticles, sol-gel.

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Non-Equilibrium Thermodynamics and Superconducting Qubit Dynamics in Kagome Latticé System

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This work presents a theoretical investigation of non-equilibrium thermodynamics in superconducting qubits based on Kagomé lattice structures. The interplay between superconductivity, geometric frustration, and topological properties unique to the Kagomé lattice, using BCS theory and Bogoliubov-de Gennes equations has been explored to describe superconducting pairing and quasiparticle excitations. The Keldysh formalism is employed to model non-equilibrium dynamics, capturing dissipation and transport effects critical to superconducting systems. Additionally, a tight-binding approach reveals the unconventional superconducting states and flat bands of the Kagomé lattice, which support robust qubit states. Using the Lindblad equation, the impact of non-equilibrium conditions on qubit coherence has been analysed, focusing on relaxation and dephasing processes that influence quantum coherence and qubit performance. This study offers insights into non-equilibrium effects and topological features for improved qubit designs in quantum computing.

Keywords: Keldysh Green function; Superconducting Qubit; Quantum Computing

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Vehicular Speed Sensor based on Au@PVDF-HP/ZnO Piezoelectric Nanogenerator

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Here we report a high-performance sensitive device capable of detecting the presence and movement of wheels. The Au nanoparticles as nanofiller were incorporated in the PVDF-HFP matrix and drop cast on hydrothermally grown ZnO resulting in electrode-composite film-electrode stack configuration. The X-ray diffraction study and Fourier transform infrared (FTIR) spectroscopy of the composite film confirms significant enhancement in the β-phase crystallization within the PVDF-HFP matrix, attributed to the incorporation of Au nanoparticles. At optimum Au concentration, the device generated an output voltage of about 13 V and exhibited a maximum power of $\sim 25\ \mu W / (cm^2)$ at an external load of 1300 KΩ and charged a commercially available capacitor of 0.22μF up to $\sim 1.28\ V$ in just 14s of operation. This ZnO/Au@PVDF-HFP composite nanogenerator demonstrated good sensitivity to human motion. Finally detecting the presence and movement of wheels was demonstrated using a two-wheeler. Therefore, this ZnO/Au@PVDF-HFP system has the potential to serve as a foundation for future low-cost, highly sensitive smart vehicular movement detection combined with efficient energy harvesting.

Keywords: ZnO, PVDF-HFP, Piezoelectric, Nanogenerator

Low-Cost Planar Microwave Sensor for Permittivity Analysis and Adulteration Detection

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This work presents a low-cost planar microwave sensor for dielectric characterization and adulteration detection of samples. The sensor is designed using Ansys High Frequency Structure Simulator (HFSS) software on a commercially available FR4 substrate of thickness 1.6 mm. The sensor design comprises of two identical resonators excited by a common 50Ω transmission line which provides differential excitation to the resonator structure. The proposed differential sensor works on the principle of frequency splitting which arises due to the mismatch of capacitance of the resonators due to the presence of a dielectric sample. Also, the same sensor can be used as a comparator which can determine the variation of a sample from its pure state to an adulterated state. Using multiple samples, the performance of the sensor is evaluated and empirical fitting equations have been developed from which an unknown sample is characterized which high accuracy. The sensor promises to be a potential candidate for high sensing applications with the advantage of differential sensing despite being a low-cost option.

Keywords: Microwave sensor; frequency splitting; differential; permittivity

Poster Presentation

Structural, Optical and Magnetic Properties of Holmium-Cobaltites

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The physical properties of Rare-earth based Perovskites oxides (ABO_3) have been studied widely over the past few decades because of their interesting physical phenomena [1]. Especially their novel magnetic and electronic transport properties have important applications in the field of magneto electronic devices [1,2]. Some vital features of these compounds include magnetic field induced first-order meta-magnetic transitions, colossal magnetoresistance, charge ordering, metal-insulator transition etc., [3]. Such properties usually arise from complex interplay of all quantum variables that interact with each other to determine the physical properties of materials like spin, charge and orbital degree of freedom and lattice deformations. In this context here, we report a unique combination of the Holmium based cobaltite perovskites of stoichiometry $Ho_{1-x}Ca_xCoO_3$ (HCCO) with compositions x = 0.2, 0.5, 0.8 and 1. Effect of Ca substitution as well as the role of sintering temperature on formation, crystal structure, optical and magnetic properties of HCCO are studied in detail by various characterization techniques. The Rietveld refinement technique using X-ray powder diffraction data reveal orthorhombic perovskite-type structure with the *Pbnm*- space group. The optical energy bandgap (E_G) estimated form the UV-Vis-NIR spectra through diffusive reflectance spectroscopy by employing Kubelka-Munk method (Fig.1c,d) reveal a strong dependence on Ca substitution level ($2.5eV \leq E_G \leq 1.63$ eV). The temperature dependence of magnetization data reveals very weak ferromagnetic nature with Curie temperature TC ~ 2.77 K (Fig. 1a). The temperature dependence of the magnetic susceptibility $\chi(T)$ of HCCO (for x = 0.2) is mainly determined by the spin moment of rare-earth Ho ions and the additional paramagnetic contribution induced by the thermally excited trivalent Co magnetic terms having multiplet splitting into Kramers sublevels (Fig. 1b).

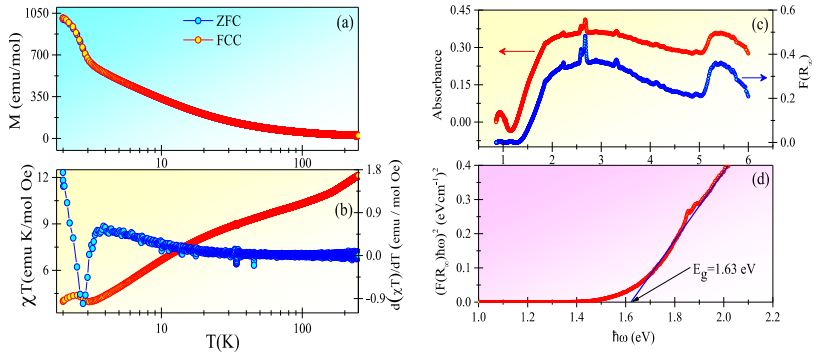

Fig. 1: (a) Magnetization Vs. Temperature of $Ho_{1-x}Ca_xCoO_3$, x = 0.2 and the corresponding (b) differential susceptibility plots ($d(\chi T)/dT$) obtained from the χT Vs. T. Energy ($\hbar\omega$) variation of (c) optical absorbance and (d) Kubelka-Munk (KM) function $[F(R\infty)(\hbar\omega)]^2$ yielding the energy bandgap E_G ~1.63eV.

Keywords: Perovskites; Ferromagnetism; Kramers sublevels; Rietveld refinement.

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Magnetically Recoverable Zinc Ferrite Nanoparticles as Highly Efficient Heterogeneous Catalysts for *Ipso*-Hydroxylation Reaction

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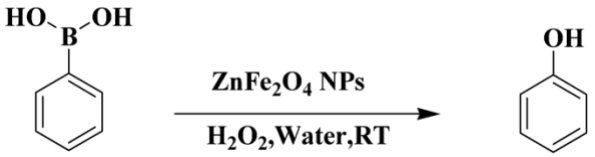
Zinc ferrite magnetic nanoparticles have demonstrated exceptional catalytic efficiency for the *ipso*-hydroxylation reaction in aqueous media at ambient temperature, eliminating the need for stringent reaction conditions. Their intrinsic magnetic properties render these bimetallic nanoparticles highly effective as heterogeneous catalysts, facilitating effortless separation and regeneration. The catalyst can be readily recovered via an external magnet without compromising yield, maintaining catalytic activity over five consecutive cycles. This methodology presents significant advantages, including facile recyclability, reduced reaction times, high product yields, and operation under mild conditions, making it an attractive approach for sustainable catalysis.



Scheme: Synthesis of phenol using $ZnFe_2O_4$ MNPs.

Keywords: High yield; Short reaction time; Magnetically separable & recyclable

Reference:

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NO Adsorption Behaviour on Defective MgO monolayers

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The development of miniaturized, highly sensitive, and selective gas sensors with rapid response times is crucial for applications in environmental monitoring, food safety, and industrial automation [1]. Crystalline two-dimensional (2D) materials are particularly promising due to their high surface-to-volume ratio and numerous reactive surface sites, allowing even minimal gas adsorption to significantly alter electronic conductivity. Nitric oxide (NO) is one of the most common toxic gas commonly emitted by industries and vehicles, and its increased concentrations can result in acid rain [2]. Therefore, detecting NO gas is crucial for maintaining a healthy living and working environment. Motivated by this fact, a density functional theory (DFT) based study has been performed on graphene-like hexagonal pristine and defective MgO(111) monolayers (MLs) for the molecular adsorption of NO. The study investigates the role of Mg and O vacancy defects on structural, electronic, and gas-sensing properties of MgO ML associated with the adsorption of NO. All the monolayers are semiconducting with magnetic behaviour shown by that in presence of Mg vacancy defects. Adsorption of NO molecule leads to a reduction in the electronic energy bandgap of the MLs and there is emergence of magnetic properties for all of them. The computed adsorption energy indicates that NO adsorption becomes stronger in the vacancy-containing monolayers compared to the pristine MgO ML. The calculated work function values support the nature of NO interaction in the studied systems. Relative to the ultra-fast gas sensing response in pristine ML, large recovery time in the defective monolayers facilitates the NO gas removal applications.

Keywords: DFT; MgO monolayer; Adsorption; Work function; Recovery time.

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Exploring the Tracking of Microparticle Diffusion in Electrolytic Media: Brownian and Anomalous Diffusion

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This work explores the diffusion behaviours of microparticles in electrolytic solutions, aiming to determine whether their motion follows classical Brownian motion or demonstrates characteristics of anomalous diffusion. These diffusion patterns are fundamental to fields such as soft matter physics, colloidal systems, and bio-applications, where the transport of particles is crucial. While the concept of Brownian motion is well understood [1], the phenomenon of anomalous diffusion-arising from more complicated interactions in electrolytic environments-remains an active area of study [2].

In this experiment, polystyrene microparticles are suspended in various electrolytic solutions, such as deionized water, saline, and phosphate buffer, each presenting different ionic strengths. The motion of these particles is recorded using advanced microscopy techniques, enabling both image and video capture [4]. To distinguish between Brownian and anomalous diffusion, the Mean Squared Displacement (MSD) analysis is applied, allowing for a precise quantification of particle movement [2].

The outcomes of this investigation tend to enhance the current understanding of how microparticles diffuse in electrolytic media, particularly in identifying deviations from classical Brownian motion [1, 2]. These findings are also anticipated to be relevant in biological systems, particularly in the transport of nanoparticles through lipid membranes and ion channels [3]. The insights gained could be instrumental in the design of more effective drug delivery systems and medical devices. This work aims to address the complexities involved in particle diffusion within electrolyte-rich environments and could have significant applications in both technological and biological domains.

Keywords: Microparticle diffusion, Electrolytic media, Brownian motion, Anomalous diffusion

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Highly Selective Solution and Film based Sensor for Colorimetric Sensing of Arginine in Aqueous and Blood Samples

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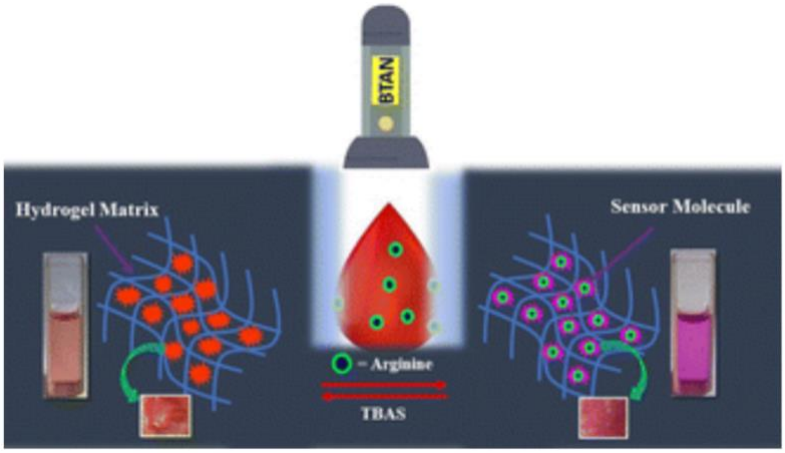
Arginine is a vital amino acid involved in various physiological processes, including nitric oxide synthesis and immune response. Alterations in arginine levels have been linked to several health conditions such as cardiovascular diseases, metabolic disorders, and immune dysfunctions. Accurate and sensitive detection of arginine in biological fluids like blood is critical for early diagnosis and monitoring of these conditions. Traditional methods for arginine detection involve complex analytical techniques which are often time-consuming and expensive. Therefore, developing a simple, cost-effective colorimetric sensor could be a valuable tool for rapid arginine detection in clinical and diagnostic settings.

We have designed and synthesized a benzothiazole-azo based optical sensor for arginine among other 12 naturally available amino acids in semi aqueous media i.e. DMSO-H_2O (1:1, v/v). It was quite fascinating to see the rapid colour change from orange to pink on addition of arginine within 2-3 seconds which was easily discernible by naked eye. The detection limit for arginine was as low as 0.7 μM. The sensor's detection process, studied using 1H-NMR and UV-vis spectroscopy, based on deprotonating the -OH group of BTAN when it interacts with arginine, causing a visible colour change. For practical use, BTAN was immobilized into a starch-PVA hydrogel and paper strips, allowing effective on-site detection in fully aqueous environments. The sensor also showed excellent ability to avoid interference from other amino acids, which is uncommon in amino acid sensors. Additionally, the sensor was successfully tested for detecting arginine in human blood samples, offering a fast, easy, and versatile method for both qualitative and quantitative arginine detection.



Keywords: Arginine; Benzothiazole-azo; Colorimetric sensing; Hydrogel matrix.

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Altered Magnetic Order Parameters and Optical Energy Bandgap in Mn Substituted Nickel Chromate Spinels

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Among many spinels oxides (AB_2O_4) that crystalline in cubic symmetry of space group *Fd-3m,* Nickel Chromate spinel, $NiCr_2O_4$ (NCO) exhibits unique properties in which the both tetragonal (*I4₁/amd*) as well as cubic phases have been realized depending upon the synthesis conidtions [1]. In NCO the divalent Ni ions occupy the tetrahedral (A) sites and the trivalent Cr ions reside in the octahedral (B) cage of spinel lattice [1]. The introduction of Mn into the octahedral sites usually leads to a significant tetragonal distortion due to Jahn-Teller (JT) effect which is the topic of current research work. In the present study, we focus on the impact of Mn substitution on the magnetic and optical characteristics of three different levels of the Mn substitution leading to the compositions (*i*) $NiCr_2O_4$, (*ii*) $NiCrMnO_4$, and (*iii*) $NiMn_2O_4$. Preliminary crystal structure analysis based on the Rietveld refinement of the x-ray diffraction data reveals that all these three compositions are having stable cubic structure at 300 K belonging to the *Fd-3m* space group. It is noteworthy that our observations indicate that while the initial compounds, $NiCr_2O_4$ and $NiMn_2O_4$, do not exhibit substantial peak splitting (pertaining to tetragonal splitting), however, the splitting of Bragg peaks becomes more pronounced for intermediate compositions characterized by a high concentration of Mn. Such peak splitting can be ascribed due to the JT distortion effects caused by the presence of Mn^{3+} ions. All the three systems essentially show ferrimagnetic (FIM) behavior due to the imbalance in the magnetic moments of cations with FIM Néel temperature (T_{FN}) ranging from 73 - 118.6 K which is very sensitive to the level of substitution of Mn ions. The optical energy bandgap determined from the Kubelka-Munk analysis of optical reflectance was found to be decrease monotonically from 2.06 - 1.16 eV with increasing the Mn content. A systematic correlation between the structural, optical, and magnetic properties will be discussed in detail.

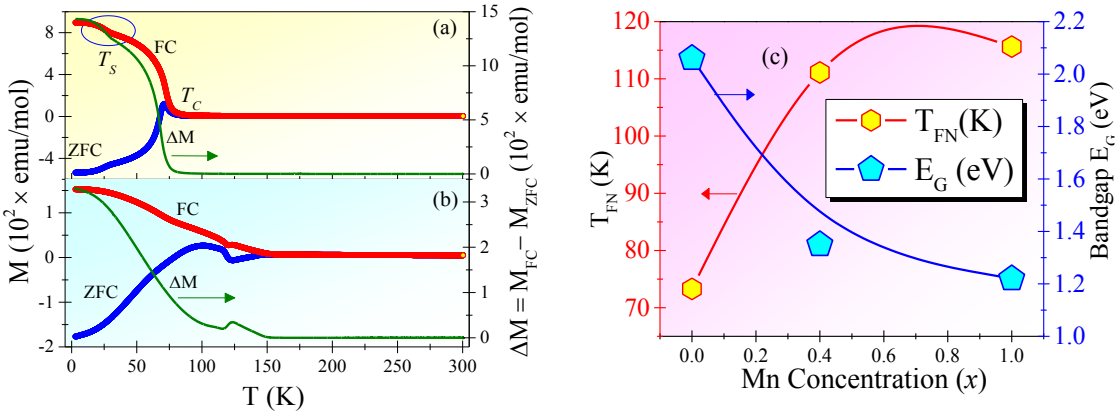

Fig. 1: (a,b) Magnetization Vs. Temperature of $NiCr_2O_4$ (x = 0) and $NiCrMnO_4$ (x = 0.5), and (c) The variation of energy bandgap, E_G and T_{FN} plotted for different levels of Mn composition.

Keywords: Jahn-Teller distortion, Kubelka-Munk analysis, Ferrimagnetic, Néel temperature.

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Highly Efficient Photo-Electric Behaviour of Carnosine dye based Synthetic DSSC incorporated with Zinc-Oxide Nanoparticles

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In recent years, dye-sensitized solar cells (DSSCs) have gained significant attention due to their cost-effectiveness, environmental benefits, and potential for high efficiency in solar energy conversion. Among the various components of DSSCs, the choice of dye and semiconductor materials plays a critical role in determining the overall photoelectric performance. This study uses Carnosine (CS), a naturally occurring dipeptide composed of beta-alanine and histidine, as a sensitizer. Its exceptional light-harvesting capabilities and stability under solar irradiation make it an ideal candidate for DSSC applications. The CS dye has been synthesized by the diazotization of $NaNO_2$ in the presence of HCl and coupling reactions by NaOH solution. The synthesized nanoparticles were validated through X-ray diffraction (XRD) analysis, found to be cubic structured nanoparticles, and confirmed by the Energy Dispersive X-ray (EDX) analysis. The fabrication process of the DSSC involves synthesizing ZnO nanoparticles (NPs) via a hydrothermal method to ensure high crystallinity and optimal size for maximum surface area. The NPs are then blended with CS dye using the surface modification process. The Composites (CPs) are then deposited onto ITO substrate to form the photoanode followed by a metal plate as the back electrode. The NPs-Dye composites were also validated with XED and SEM analysis. When combined with ZnO (NPs), the carnosine dye enhances light absorption across a broad spectrum, which in turn increases the efficiency of electron transfer from the dye to the semiconductor material. ZnO, with its wide band gap and superior electron transport properties, serves as an efficient semiconductor that improves the collection of photo-generated electrons, reducing electron-hole recombination and increasing the overall efficiency of the cell.

The performance of the carnosine dye-based DSSC in the presence of NPs is evaluated under standard solar illumination conditions. Results show a marked improvement in the overall photoelectric conversion efficiency (0.246) compared to traditional DSSCs. The enhanced efficiency is attributed to the synergistic effect of the carnosine dye and ZnO NPs. The dye's broad-spectrum light absorption, coupled with the excellent electron transport capabilities of ZnO, leads to a significant increase in the short-circuit current density (0.950 to 2.563 mAm^{-2}) and open-circuit voltage (0.25 to 0.34 V). Also, ZnO helps to reduce the average barrier height (3.867 to 2.858 eV) for better charge injection at the interface (Figure 1). Furthermore, the introduction of ZnO NPs helps mitigate charge recombination by reducing the trap distribution, contributing to an overall increase in power conversion efficiency (PCE). Also, the incorporation of ZnO increases the stability of PCE for a longer time (Figure 2) make a more valuable contribution to the application as DSSC.

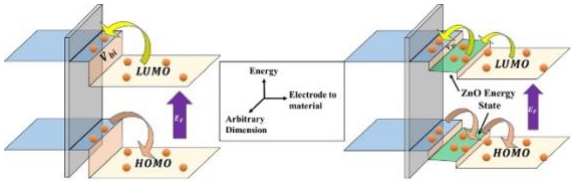

Fig. 1: Energy diagram of dye with and without ZnO NPs

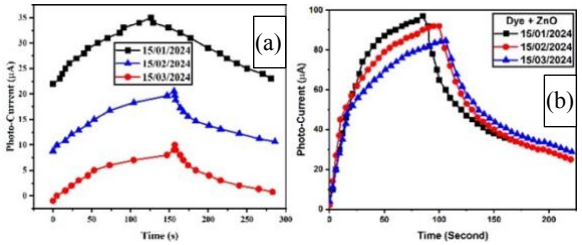

Fig. 2: Photo-Electric Stability of (a) Dye and (b) Dye with NPs

Keywords: Sunset Yellow Dye; Zinc Oxide Nanoparticles; Photo-Electric Stability; Energy state and Barrier Inhomogeneity

Electrochemical Performance and Enhanced Magnetoresistance of Self Doped $La_{0.6}MnO_{3\pm\delta}$ Perovskite for Energy Storage and Magnetic Field Sensor Applications

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Lanthanum Manganites are the highly demanding materials in the field of supercapcitor and magnetic field sensor. In this article self-doped Lanthanum Manganites was prepared for the first time by simple sol-gel method and annealed at different temperature. The prepared samples were characterized by the various techniques like XRD, FTIR, FESEM, TEM, BET and XPS. Among the different annealed compound (800^0; 900^0 *and* 1300^0C), the compound annealed at 800 ^0C shows maximum supercapacitive and magnetoresistive performance. The specific capacitance of *LMO*800 was found to be 469 *F/g* at 1 *mV/s* from Cyclic Voltammetry (CV) and 286 *F/g* at 1 *A/g* from Galvanoststic Charge Discharge (GCD) measurements, whereas *LMO*1300 shows 344 *F/g* and 106 *F/g* under the identical conditions. Wide working potential window of 2.4 *V*, 71.2 $W\ h{:}kg^{-1}$ energy density at 1 *A/g* specific current and power density of 6 *kW/kg* at 10 *A/g* specific current was achieved when a symmetric supercapacitor device was made using *LMO*800 compound. Further, the same sample shows a better cyclic stability (140% retention of specific capacitance after 5000 GCD cycles). The study of materials exhibiting large magnetoresistance (MR), which refers to the percentage change in electrical resistance when an external magnetic field is applied, a vibrant area of research for a considerable period. Apart from specific capacitance, giant magnetoresistance (MR) has a wide range of practical applications, particularly in magnetic field sensor technology. Our experimentally observed results are explained as a function of particle size of the prepared compounds, which is well agreed with the results of CV and GCD measurements.

Keywords: Perovskite, Manganite, Energy Storage, Magnetoresistance

Design and Simulation of n-WS_2/c-Si(p) Heterojunction Solar Cells using TCAD Sentaurus

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Recently, 2D semiconductors have been used with conventional bulk semiconductors to create more affordable solar cell devices because of their distinct optical, electrical, and mechanical capabilities. Out of all these materials, WS_2 demonstrated a promising potential for use in solar cell devices. In this study, we have used Technology Computer Aided Design (TCAD) Sentaurus simulation tool for modelling the device structure. We have used WS_2 thin film of 30 nm as emitter layer with c-Si(p) as absorber layer and Silver (Ag) as back electrode. Indium Tin oxide (ITO) acts as a transparent conducting oxide placed on top of WS_2 aiding in collection of photo generated charge carriers.

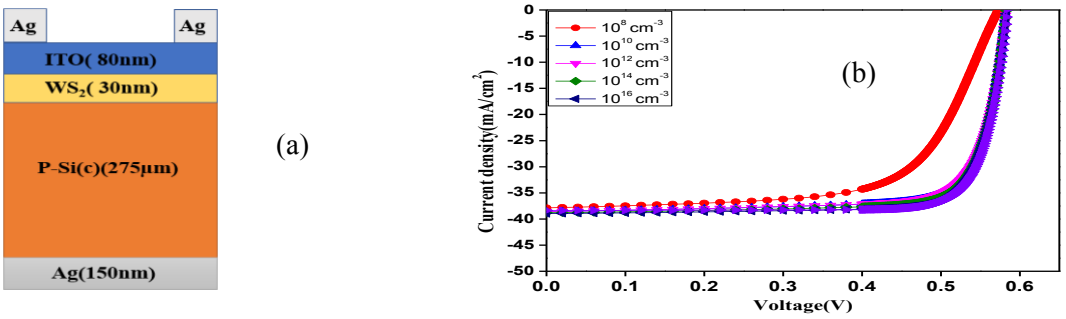

Fig. 1: (a) Device structure considered for n-WS_2/c-Si(p) heterojunction solar cell (b) The light J-V curve for different WS_2 electron concentration

The role of varying electron concentration from 10^8 cm^{-3} to 10^{16} cm^{-3} of WS_2 emitter layer on the performance parameters of device was studied and been tabulated in table 1 with their corresponding J-V curves in figure 1(b).

The results showed that with the increase in doping concentration there is a significant change in the fill factor (FF) from 0.66 (10^8 cm^{-3}) to 0.80 (10^{16} cm^{-3}) without much change in the short circuit current density (J_{sc}), which results in increase of the solar cell efficiency up to 18.17%.

Table 1: Performance parameters of the device with respect to varying WS_2 electron concentration

WS_2 electron Concentration (cm^{-3})	J_{sc} (mA/cm^2)	V_{oc} (V)	Fill Factor (FF)	Efficiency (%)
10^8	37.87	0.57	0.66	14.17
10^{10}	38.58	0.58	0.78	17.53
10^{12}	38.58	0.58	0.78	17.53
10^{14}	38.81	0.58	0.79	17.88
10^{16}	38.97	0.58	0.80	18.17

Synthesis and characterization of sodium and potassium based salts for the single-ion conducting polymer electrolytes

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Energy storage technologies are pivotal for the transition to a sustainable and resilient energy infrastructure. Electrochemical energy storage systems, such as batteries and supercapacitors, play a vital role in delivering portable power for various technological applications, including laptops, smartphones, electric vehicles, military electronics, pacemakers, and numerous other devices. Over the past few decades, lithium-based batteries have dominated the electrochemical energy storage field. However, challenges such as limited lithium availability, the use of flammable organic solvents, dendrite formation, and the short lifespan of conventional electrolyte-based batteries have necessitated the development of alternative solutions. One promising approach involves the development of sodium and potassium based single-ion conductors for energy storage applications. This study presents the synthesis of two cost-effective and environmentally friendly polymeric salts, sodium poly tartaric acid borate (NaPTAB) and potassium poly tartaric acid borate (KPTAB), using the aqueous phase separation method. These salts remained in a gel state at ambient conditions and exhibited a crystalline structure after vacuum drying. The synthesis of the polymeric salts was confirmed through NMR spectroscopy. Additionally, functional group identification, polymer-salt interactions, and surface morphology are investigated using FTIR and SEM analyses.

Keywords: Polymeric salt, sodium and potassium ion, polymer electrolytes, single-ion

Synthesis and Study of Zinc Vanadate nanostructures as photocatalyst for degradation of Methylene Blue Dye

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The study of transition metal vanadates is attracting increased attention due to their diverse structural chemistry, high density and economic viability [1]. With simple production methods, low toxicity and a small environmental footprint, these materials have found uses in fields like catalysis, optical technology, magnetic systems and energy-related applications [2]. In this work, nanostructured Zinc Vanadates (ZV NS) were synthesized via a simple co-precipitation method and subjected to calcination at different temperatures ranging from 100-600°C. Various analytical techniques were employed to evaluate the structural, morphological and optical properties of the prepared ZV samples. X-ray diffraction (XRD) analysis revealed a hexagonal phase of $Zn_3V_2O_7(OH)_2(H_2O)$ and cubic $Zn_3V_2O_5$ at lower calcination temperatures, while higher temperature samples showed orthorhombic $Zn_3(VO_4)_2$ structure. The crystallite size, calculated using the Scherrer equation, was approximately 42 nm. Scanning electron microscopy (SEM) showed agglomerated flaky morphology, whereas high resolution transmission electron microscopy (HRTEM) revealed the formation of ZV NS with crystal planes corroborating XRD studies. Fourier transform infra-red spectroscopy (FTIR) discloses various functional groups of ZV in the prepared samples. Energy dispersive X-ray spectroscopy (EDX) study reveals the elemental composition of the prepared samples to be in the ratio of 13:30:56.The band gaps of the samples were estimated to be in the range of 2.90-2.96 eV from ultra violet -visible (UV-Vis) transmittance data using Tauc plot. This higher band gap compared to the bulk counterpart is due to the formation of nanostructured ZV. Photoluminescence spectra showed strong visible light emission, peaking at 576 nm, emphasizing the potential of prepared material in visible light applications. These prepared ZV NS yield good photocatalytic degradation of dye Methylene Blue in water performed under visible light assessed using UV-Vis absorption spectroscopy. The results suggest the ZV photocatalyst is a promising, sustainable solution for removing dye pollutants from contaminated water.

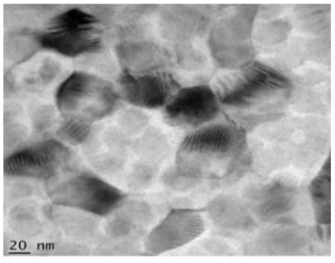

Fig.1: TEM image of ZV

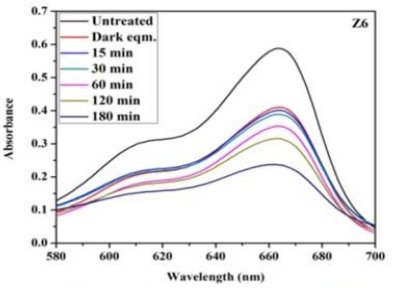

Fig.2: Photocatalytic dedegradation of MB dye

Keywords: Zinc Vanadate NS; Photocatalysts; Degradation; Methylene Blue.

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Effect of co-substitution of Al and Cr on Structural and Dielectric Properties of Cobalt Magnesium Ferrite

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Polycrystalline samples of $Co_{0.5}Mg_{0.5}Fe_{2-2x}Al_xCr_x$ (x=0-0.15) have been prepared using conventional sol-gel method. X-ray diffraction analysis confirmed the formation of single-phase spinel. Rietveld refinement of the obtained XRD patterns was done using FullProf software. Contraction of unit cell was observed upon substitution of Al^{3+} and Cr^{3+} on Fe site due to their comparatively lesser ionic radii. FTIR spectroscopy revealed the frequency data for respective sites. Raman peaks were analysed to extract the information about chemical bonding. Microstructure of the samples were analysed using Scanning Electron Microscopy and particle size were estimated from the micrographs. EDX analysis confirmed the chemical composition of the substituted samples.

The dielectric characteristics of the samples were determined by analyzing the impedance spectroscopy data. Analysis of the impedance data (Z' and Z") revealed negative temperature coefficient of resistance throughout the measured temperature range for all the samples. Study of dielectric constant and AC conductivity data followed the similar trend. Modulus spectrum analysis confirmed the thermally activated sample-electrode effects. The AC conductivity data of the samples were found to follow Jonscher Power Law (JPL).

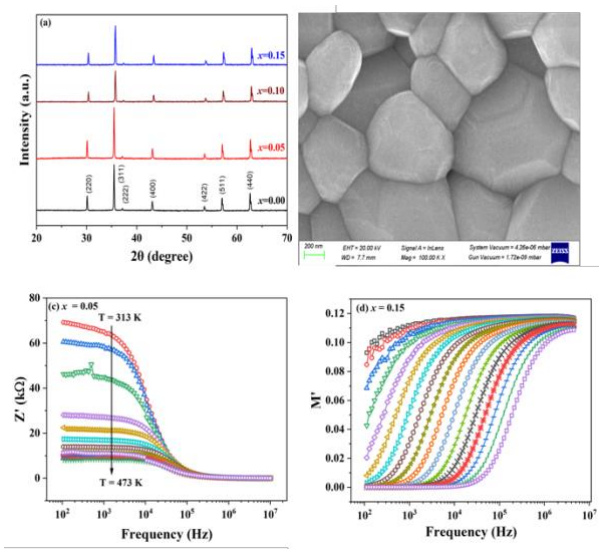

Fig. 1: (a) Room temperature XRD patterns for all samples, (b) SEM micrograph for x = 0.00 sample, (c) Z' vs frequency for x = 0.05 sample, (d) M' vs frequency for x = 0.15 sample.

Keywords: Sol-gel method; Spinel; Impedance spectroscopy; AC conductivity

Self-action Effect in Negative Index Material

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Negative index meta-materials are known for its exotic and unique electromagnetic properties, that includes negative refraction, not observed in naturally available conventional materials. Researches in negative index meta-materials grew in leaps and bounds since the demonstration of negative refraction in 2001 by Smith et.al. in a wedge shaped meta-material prism that comprised of a combination of wires and split-ring resonator(SRR). The proprieties of these materials can be tailored by adjusting the dimension, periodicity etc., of "meta-atoms" - the constituent engineered micro-, nano- structures, for varied applications like invisible cloak, seismic wave dampener, sound wave absorber etc. In the domain of non-linear optics these materials enable new phenomenon and has the capability of "revolutionizing non-linear optics, enabling new generation of non-linear devices for optical and quantum communication, optical computing, and image processing".

In context of the above background this study investigates the spatial behaviour of a laser beam propagating in a representative negative index material(NIM) with beam power $P \geq P_{cr}$, the critical power using the non-linear Schrodinger equation (NLSE). The results are obtained solving NLSE with variational method, focusing chiefly on non-linear optical self -action effects. These phenomena in negative index material are yet to be fully explored. The results of the study indicate self- focusing cannot be observed in NIM as long as the non-linear refractive index in NIM, $n_2 > 0$.

Keywords: Negative index material; Negative refraction; Exotic optical properties; Self - focusing

Exploring Lightweight High Entropy Alloys for Radiation Resistant Applications

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High entropy alloys (HEA) are considered as multicomponent alloys having at least five major metal elements, each having an atomic percentage of 5–35%. HEAs show extraordinary properties such as good corrosion and oxidation resistance, friction and wear resistance, high strength and hardness, good structural stability, irradiation resistance etc. To predict the phase stability of the HEAs a quantitative analysis is generally done with the help of various physical and thermodynamic parameters namely: the atomic size difference (δ), the mixing enthalpy (ΔH_{mix}), omega parameter (Ω), the electronegativity difference ($\Delta\chi$) etc. The single-phase formation rules for these parameters are given as: $\delta < 6.6$, $-15\ kJ/mol \leq \Delta H_{mix} \leq 5\ kJ/mol$, $\Omega > 1.1$, $\Delta\chi \leq 0.175$. [1],[2].

Here we explore a few optimistic light weight high entropy alloys following analytic and quantitative rules. The lightweight high entropy alloys (LHEA) composed of light main group elements such as Al, Mg, Li, Ca etc. LHEAs are in a very early stage of exploration having a great potential to be used in various lightweight material fields such as aerospace technology. They have the potential to show superior mechanical and radiation resistant properties with good structural stability compared to the existing lightweight materials. [3]. LHEAs have great potential to be used in various radiation resistant applications due to their highly distorted lattice structure which resists the movement of dislocations and various defects produced in the material during the irradiation process. [4].

After careful analysis we have found that in case of AlCrMgSiZn alloy, the elements Al, Cr and Zn profoundly contribute to the formation of single phase while Si and Mg are responsible for the development of multiphase and amorphous phases. Moreover, with the replacement of Si by Mn (AlCrMgMnZn alloy), the formation of single-phase structure can be predicted for all the equiatomic and non-equiatomic compositions. The theoretical densities were also calculated for the two alloys using the rule of mixture assumption and found the density to lie between 3 to 5.5 g/cm^3. The phase stability analysis along with the basic properties of the HEAs will be elaborated in this presentation.

Keywords: High entropy alloy; Phase stability; Radiation resistance

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Computational Study of the Hydrolysis Reactions of the Ground and First Excited Triplet States of Bare and Transition Metal Doped Ti_2O_4 Cluster

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In the field of renewable energy, hydrogen (H_2) has been considered a promising energy carrier that has the potential to replace current fossil fuel-based energy sources. Hydrogen is a clean, renewable fuel that has the potential to be a future energy carrier. A large reduction in carbon emissions can be obtained by manufacturing hydrogen using renewable energy sources. Green hydrogen is a clean and sustainable energy source that causes significantly lower greenhouse gas emissions. Transition metal oxides, such as zinc oxide (ZnO), titanium dioxide (TiO_2), ruthenium dioxide (RuO_2) etc., have potential applications for the water splitting reaction (WSR) process. Density functional theory (DFT) method is used to investigate the formation of H_2 and O_2 molecules from hydrolysis products formed by H_2O addition to metal oxide clusters. In this regard, we have performed hydrolysis reactions of the ground and first excited triplet states of bare and transition metal-doped Ti_2O_4 clusters to accomplish the WSR process in the future.

Fig. 1: Hydrolysis of Ti_2O_4 and Zirconium-doped Ti_2O_4 clusters.

Keywords: Green hydrogen; Water splitting reaction; Metal oxides; Density functional theory

Investigation of Ag-Doping Concentration on the Optical and Structural properties of ZnS nanostructured thin films for Photovoltaic Applications

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Semiconductor nanomaterials from the II–VI group have garnered significant attention over the past few decades, owing to their distinctive optical and luminescent characteristics [1]. Zinc sulfide (ZnS), a well-known binary compound semiconductor within this group, is widely used in various electronic and optoelectronic applications [2,3]. While semiconductor nanocrystals possess remarkable characteristics, their properties can be further enhanced through doping with transition metals (TMs). Among these, group I metals such as silver (Ag) and copper (Cu) are recognized as fast-diffusing impurities in II–VI compounds [4]. In this study, nanostructured ZnS thin films doped with varying concentrations of Ag (1%, 3%, 5%, and 7% by volume/volume ratio) were synthesized using a solvent casting method followed by a thermolysis technique. The optical, structural, and compositional properties of the films were analysed using UV-Visible spectroscopy, X-ray diffraction (XRD), high-resolution transmission electron microscopy (HRTEM), scanning electron microscopy (SEM), and energy-dispersive X-ray analysis (EDAX). XRD results indicate that the intensity of the diffraction peaks increases with Ag doping concentration, suggesting an enhancement in the crystalline quality of the films. The films exhibit a nanocrystalline nature with a cubic phase, showing preferred orientations along the (111), (220), and (311) planes up to a 5% Ag doping concentration. At 7% Ag doping, a hexagonal peak corresponding to the (100) plane emerges. Additionally, the d-spacing values increase with Ag doping concentration, as confirmed by both XRD and HRTEM analyses. Optical characterization reveals a slight decrease in transparency and a red shift in the absorption edges with increasing Ag concentration. These findings emphasize the significant impact of Ag doping on the structural and optical properties of ZnS thin films, paving the way for potential applications in advanced electronic and optoelectronic devices.

Keywords: Zinc Sulphide; Thin film; Nanostructured; Silver-doping; X-ray diffraction

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Two dimensional V_2S_2 as an Efficient Anode Material for Alkali Metal Ion Batteries

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This study investigates a proper anode for alkali metal-ion batteries (MIBs) in response of urgent demand for effective devices for storing energy. The 2D V_2S_2 system can be a potential material as a MIB anode. We have employed the density functional theory formalism utilizing the generalized gradient approximation (GGA) Perdew-Burke-Ernzerhof (PBE), within the Vienna Ab Initio Simulation Package (VASP) to examine the energetical, dynamic, and thermal stability of pristine V_2S_2 monolayer sheet. To rule out the possibility of mutual interaction of the system and its periodic image, we consider a 20 Å separation along the z-axis. A k-point grid of (3×3×1) is employed for the Brillouin zone sampling following the Monkhrost-Pack scheme. Electronic band structure calculation shows that the pristine monolayer has inherent metallicity, which satisfies one of the criteria for being an electrode material. Van der Waals interactions inside composite systems with the metal adsorbed were included based on the Grimme's DFT-D3 correction. The CDD and the Bader charge analysis are done to investigate the charge transfer process. In addition, the climbing image nudged elastic band (CI-NEB) approach is taken for predicting the minimum energy pathway (MEP) in conjunction with VTST tools. The electronic and structural characteristics of the V_2S_2 systems with the adsorbates of alkali metals and the charge transfer within the system are explored. The barriers of Li, Na, and K migration are computed as 0.42 eV, 0.12 eV, and 0.14 eV, respectively. In addition, our predicted systems demonstrate a significant theoretical storage capacity of 968.9 mAh/g for the lithium and sodium atoms. The computed open-circuit voltages support that this monolayer can be a practical 2D anode. Figure 1 (a, b, c) show the plots of theoretical storage capacity plotted with alkali metal (Li, Na, and K) concentration.

Keywords: Metal-ion battery electrode; anode material; theoretical storage capacity; sodium ion battery, two-dimensional monolayer

Insight into Electric Transport and Dielectric Relaxation of Fe Doped Glassy Semiconductor

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The development of semiconducting nanocomposites, xFe-(1-x) (0.5 V_2O_5 -0.4 CdO-0.1 ZnO) is particularly important not only for exploring their microstructures using X-ray diffraction, SEM techniques, but also exploring their electrical conduction mechanism in terms of hopping of small polarons. The presence of various nanophases such as ZnO, CdO, $Cd_{9.5}Zn_{0.5}$, ZnV, $Zn_3V_2O_8$ have been identified and the size of estimated nanocrystallites is found to decrease with more incorporation of Fe content in the compositions. As the value of lattice strain increases with the increase of Fe content in the compositions, the present system becomes more and more unstable, which may be favourable for better electrical transport phenomena via polaron hopping process. Electrical conductivity of the system has been analysed using Almond-West Formalism and High frequency conductivity spectra of the present glassy system have been studied. Experimental data reveal that both optical photon and acoustical phonon transitions are responsible for the entire electrical conduction process. Polaron hopping is expected to be of percolation type, which has been validated from estimated range of frequency exponents. All experimental data have been used to frame a schematic model to explore conduction mechanism inside the present glassy system. Modulus (imaginary) plots at various temperatures reveal the dielectric relaxation process of the present system.

Keywords: Fe-doped semiconducting system; Microstructure and Surface morphology; Polaron hopping; Dielectric modulus plots

Influence of Copper Addition on the Properties of CdS/PVA Thin Films: Structural, Morphological, and Optical Analysis

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In this study, Cadmium sulfide (CdS) thin films embedded in polyvinyl alcohol (PVA) doped with varying molar concentrations of cupric nitrate solution viz. 0.5 M, 1 M, and 1.5 M were prepared using a casting technique followed by a thermolysis process. Structural analysis of the films reveals them to be polycrystalline, exhibiting a mixture of cubic and hexagonal phases. The average crystallite size, determined from the most intense XRD peak using Scherrer's formula, ranges from approximately 2.8 to 5.5 nm and decreases with increasing copper molarity. The lattice strain calculated from Williamson-Hall plot increases with increase in copper molarity. Scanning Electron Microscopy (SEM) images show that the film with 1 M copper concentration has the smoothest and most uniform surface. Optical characterization through UV-Vis spectroscopy indicates high transparency in the visible range for all films, with a sharp transmission edge suggesting good crystallinity. Both the optical bandgap energy and Urbach energy were observed to increase with higher copper molarity, reflecting changes in the film's electronic properties.

Keywords: Cadmium sulfide; Copper-doping; Solvent casting; Williamson-Hall analysis

Effect of *Dillenia indica* Plant Extract on Structural and Magnetic Behaviour of Cobalt Ferrite Nanoparticles and its Catalytic Activity for the Facile Access of Nitroarenes and Phenols

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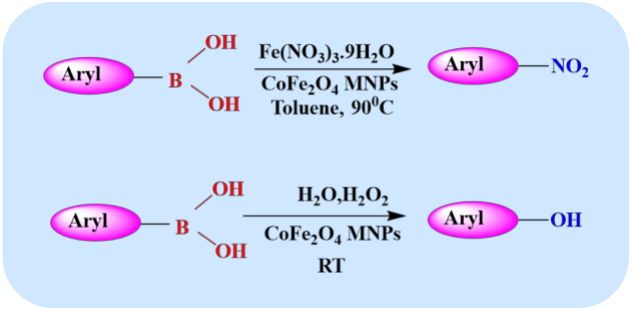
The cobalt ferrite nanoparticles, recognized for their ferromagnetic characteristics, minimal conductivity, and superior electrochemical stability, were synthesized via green synthesis route. The effect of *Dillenia indica* plant extract was explored on the structural and magnetic behaviour of cobalt ferrite samples using techniques such as SEM, PXRD, HR-TEM, EDX, IR and VSM. The SEM and HR-TEM analysis showed the variation of morphology and size of the nanoparticles in presence and absence of plant extract solution. The X-ray diffraction pattern has confirmed the cubic spinel structure of $CoFe_2O_4$ nanoparticles. VSM analysis showed change in saturation magnetization value with the presence and absence of plant extract solution.

This study explores the potential of $CoFe_2O_4$ nanoparticles as catalyst for the facile synthesis of nitroarenes and phenols. The catalytic system is highly sustainable for a great number of substrates with a high yield of product. Furthermore, owing to its magnetic nature, the catalyst demonstrated excellent recyclability without any significant loss in its efficiency.



Scheme: Application of biogenic cobalt ferrite nanocatalyst

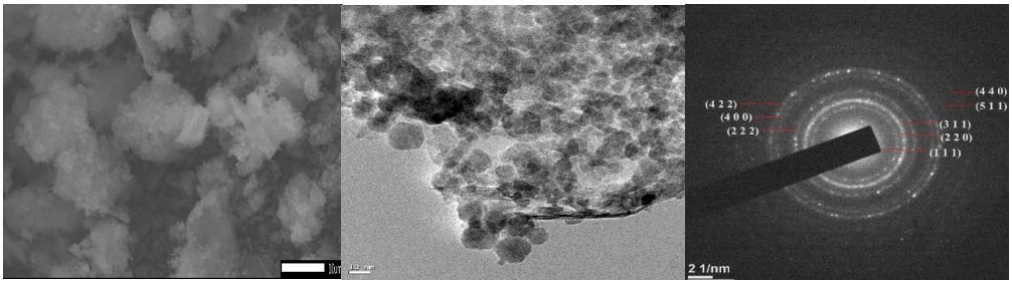


Fig. 1: (a) SEM image of $CoFe_2O_4$ NPs(b) TEM image of $CoFe_2O_4$ NPs (c) SAED pattern of $CoFe_2O_4$ NPs

Keywords: $CoFe_2O_4$ nanocatalyst; sustainable; recyclability; heterogeneous catalysis

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Magnetization Dynamics of Two Dimensional Magnetic Materials at Finite Temperature

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In this study, we investigate the magnetization dynamics of two-dimensional magnetic materials under the influence of DC and AC biasing fields using the Landau-Lifshitz-Bloch (LLB) equation. We explore the role of applied frequency, Spin-Orbit Torque (SOT), and anisotropy from a stochastic perspective. Our results show that under DC biasing, magnetization rapidly decreases at low temperatures and exhibits oscillations near the critical temperature. A potential switching effect is observed at the Landau limit, with increased oscillation at higher temperatures due to enhanced field-like torque. Under AC biasing, the system acts as a magnetization switcher in the Landau limit, and by tuning the applied frequency, it can serve as an oscillator in the moderate temperature regime. In the high-temperature region, chaotic oscillations emerge, confirmed by Maximum Lyapunov Exponents (MLE). Additionally, free energy minimization indicates the possibility of bifurcations and chaotic behaviour as temperature, anisotropy, and SOT increase, suggesting the potential for chaotic oscillations in the system.

Keywords: 2D Materials; Spin-Orbit Torque; Chaos

Plastics in Transition : A Journey from Macro to Nano-scale

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History of human progress is the history of progress in materials that has been instrumental in bringing positive changes. Since the stone age, no material has ever been so ubiquitous and omnipresent in human life like the plastics are. After the invention of Bakelite, the first synthetic plastic, millions of tons of many other plastics and their composite forms have been developed, manufactured, used and finally ended up as waste in nature. This work attempts to understand the mechanism that allows macro sized plastics to turn into nano-sized polymer clusters through an analytical and computational aspect. Additionally, the investigation extends to the fate of those nano-sized polymer clusters inside a cellular system with an emphasis on the role of nano-plastics in disrupting cellular lipid metabolism.

Keywords: Nanoplastics; Microplastics; Cellular Uptake; MD Simulation

Facile Synthesis of CeO_2 Nanocrystals and Investigation of their Microstructural and Optical Properties

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In this work, cerium oxide (CeO_2) nanocrystals were synthesized using the chemical co-precipitation process, followed by calcination at a temperature of 500 °C. The synthesized nanocrystals were characterized using X-ray diffractometer and UV-visible spectrophotometer to investigate their structural and optical properties. The Williamson-Hall and modified Williamson-Hall methods were used to analyse the physical properties such as crystallite size, strain and dislocation density of the nanocrystals. The Williamson-Hall analysis provided insights into the crystallite size and lattice strain, while the modified Williamson-Hall analysis was used to determine the crystallite size and dislocation density. We initially calculated the crystallite size using the Scherrer's formula, which yielded a value of 12 nm. However, the crystallite sizes obtained from the Williamson-Hall method and modified Williamson-Hall method were larger, approximately 17 nm. This difference suggests that the Williamson-Hall and modified Williamson-Hall methods account for additional factors, leading to a more accurate estimation of the crystallite size. The dislocation density was found to be $(7.4\pm0.5)\times10^{17}$ m^{-2} and the lattice strain was found to be $(3.48\pm0.22)\times10^{-3}$. Additionally, the optical properties of the CeO_2 nanocrystals were also studied using the UV-visible absorption spectrum and Tauc's plot. Cerium oxide exhibits an indirect band gap and from the Tauc's plot analysis, the band gap energy of the prepared materials was found to be 3.30 eV.

Keywords: Semiconductor nanostructure; Modified Williamson-Hall; CeO_2; Optical properties

Incorporation of MXene into All-inorganic Halide Double Perovskite and its Influence on Resistive Switching Behaviour

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Mxene, a novel family of 2D materials, has gained significant attention due to its excellent properties like high electrical conductivity and mobility. Meanwhile, lead free all-inorganic $Cs_2AgBiBr_6$ double perovskite (DP) has proved to be a magnificent active material for different optoelectronic applications. In our work, 2D $Ti_3C_2T_x$ MXene is incorporated as an additive in $Cs_2AgBiBr_6$ DP to investigate its effects on the structural and optical properties of the DP. The pristine $Cs_2AgBiBr_6$ is synthesized using a one-step solution-processed method and subsequently $Ti_3C_2T_x$@$Cs_2AgBiBr_6$ composite is synthesized with different $Ti_3C_2T_x$ additive concentrations, etched from its Ti_3AlC_2 MAX phase. The X-ray diffraction (XRD) pattern of the pure and $Ti_3C_2T_x$ incorporated samples shows the typical face-centered cubic (FCC) structure of the $Cs_2AgBiBr_6$ DP crystal with change in average crystallite size at different $Ti_3C_2T_x$ concentrations. The UV-vis-NIR absorption and Photoluminescence (PL) study is conducted to analyze the optical properties of the pristine and composites. The pristine $Cs_2AgBiBr_6$ DP shows an absorption edge at the visible regime with a band gap of 1.82 eV, while 2D $Ti_3C_2T_x$ incorporation causes a slight shift in the absorption edge. Additionally, changes in the PL peak intensity of the DP specifies the variation in its carrier recombination dynamics with different additive amounts. Furthermore, resistive switching study of the DP shows that $Ti_3C_2T_x$ incorporation improves the resistive switching performance by lowering the SET voltage in the fabricated memristive device. These structural and optical analyses of $Ti_3C_2T_x$@$Cs_2AgBiBr_6$ composites and its improved resistive switching behaviour indicates its potential for future optoelectronic applications with optimized additive concentration.

Keywords: Halide Double Perovskite; MXene; Composites

A Comparative Study on Structural and Optical Properties of Multilayer Cu_xO/ZnO and ZnO/Cu_xO Heterojunction Thin Films

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The present work reports the comparative study of multilayered Cu_xO/ZnO and ZnO/Cu_xO nanocomposite thin film deposited by physical vapour deposition technique. Copper (Cu) thin film was deposited by radio frequency (RF) magnetron sputtering of a metallic Cu target. Then subsequent thermal annealing was performed at 300℃ under atmospheric pressure to developed Cu_xO thin film. The ZnO layer was deposited by thermal evaporation of pure ZnO powder. Cu_xO/ZnO and ZnO/Cu_xO nanocomposite thin film were developed on glass substrate. The structural and optical properties were analysed by X-Ray Diffraction (XRD) and Ultraviolet-Visible (UV) spectroscopy respectively. The XRD pattern reveals the polycrystalline nature of the nanocomposite thin films. It also confirms the formation of three-phase nanocomposites viz: ZnO- cubic, CuO-monoclinic, and Cu_2O cubic phases. The absorbance and transmittance of the films were analyzed using UV-Visible spectroscopy. It reveals that Cu_xO/ZnO and ZnO/Cu_xO have a transmittance of about 70% and 80% respectively. Optical bandgap energy values for the Cu_xO/ZnO and ZnO/Cu_xO samples were determined from UV-visible spectrum. A systematic investigation of the change in optical bandgap and crystallite size of the nanocomposite thin films has been undertaken in this work.

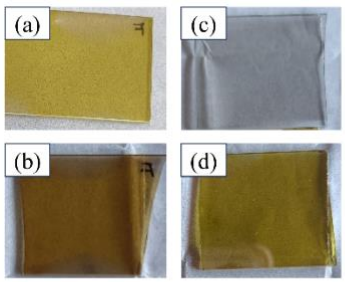

Fig. 1: (a) Cu_xO (b) Cu_xO/ZnO with ZnO as top layer. (c) ZnO (d) ZnO/Cu_xO with Cu_xO as top layer

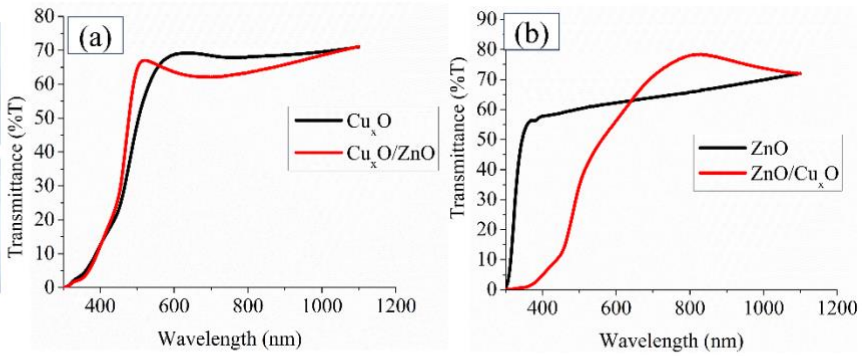

Fig.2: Transmittance spectra of (a) Cu_xO/ZnO (b) ZnO/Cu_xO

Keywords: Heterojunction, RF sputtering, X-Ray Diffraction, Thermal evaporation

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Aluminium Thin Film Mirror Fabricated by Thermal Evaporation Technique

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Aluminium (Al) is an excellent cost-effective material widely used in optical and infrared mirror technology. It has unique physical properties viz: light weight; good conductor of heat and electricity; high reflectivity etc. These propertiesuphold its candidature as reflective coating materials for car head lamps, LEDs, telescopes and interferometers.

In this work, highly reflecting Al thin film is thermally deposited on 25 mm glass substrate. The film is deposited under base pressure of ~ 10^{-5} mbar at room temperature. The current passing through the tungsten basket during thermal evaporation was maintained in the range of 1.5 - 2 A. The thin films were annealed at temperature 200 C and 400 C for 1 hour. A systematic investigation on the effect of oxide layer at air-aluminium interface to the electric conductivity of the film under different working temperature will be presented.

Fig. 1: (a) Experimental set-up

Fig. 1: (b) Aluminium mirror

Keywords: High reflectivity; thin film; thermal evaporation; electric conductivity.

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[3] P.Katiyar et al., *ActaMaterialia*, 53 (2005) 2617-2622.

Combinational Therapy against MDA-MB-231 Cell Line Using A HSP90-Inhibitor and Doxorubicin Encapsulated Nanocubes

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As a unique population of breast cancer, triple-negative breast cancer (TNBC) have been implicated in relapse and chemoresistance for lacking oestrogen receptors, progesterone receptors and HER2 amplifications. Therefore, understanding the chemoresistance cells can pave the way for introducing novel molecular targeted nanoparticle-based therapies for treating TNBC patients. Among nanoparticle based therapy, Prussian blue nanocubes have shown efficient results with appropriate biocompatible property in TNBC. In chemoresistance mechanisms, HSP90 is a crucial marker and conserved molecular chaperone that regulates the stability, activation and maturation of more than 200 client proteins including receptor transcription factors (CD44), signalling proteins (TP53, BAX/Bcl-xl) and also associated with poor prognosis and worse recurrence-free survival in TNBC. To resolve the HSP90 based chemoresistance mechanisms, Gd@mSiO$_2$@HA@DOX@ novobiocin has been developed with PDT and PTT effect. The Gd@mSiO$_2$@HA@DOX@ novobiocin when delivered within the cell will release both the drugs which will inhibit the formation of HSP90 and downregulate MDR in the system which will show better therapeutic efficacy than individual treatment method. The purpose of this study Gd@mSiO$_2$@HA@DOX@ novobiocin enhancing mild-temperature enhances PTT with a high efficiency of photothermal conversion (37.83%), PDT along with MRI effect. The cytotoxicity Gd@mSiO2@HA@DOX@ novobiocin is 18.60 µg/mL that regulates apoptosis mechanisms along iROS production in MDA-MB-231 cells. In similar dose of Gd@mSiO$_2$@HA@DOX@ novobiocin, the markers CD44, HSP90, TP53, and MDR1 will be downregulated that will maintain chemoresistance mechanisms in MDA-MB-231 cells. Such a nanoparticle will enhance cell death and downregulate HSP90, thus enhancing PTT and moderately reducing drug resistance, ultimately enhancing better therapeutic strategy and delivery of co-drugs in MDA-MB-231 cells.

Keywords: Novobiocin, HSP90, MDR1, Co-drug delivery

Ag Nanoparticles Decorated $NiFe_2O_4$ Binary Magnetic Nanocomposite for the Hydration of Aromatic Nitriles to Primary Benzamides

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Magnetic nanocomposites (MNCs) as catalysts offer a promising catalytic system that create a bridge between heterogeneous and homogeneous catalysis, integrating the facile separation of heterogeneous catalysts with the adjustability of homogeneous counterparts. Transition metal-catalysed hydration of nitriles represents a pivotal route to amides, which is a crucial synthetic building block in both industrial and academic settings. Numerous heterogeneous and homogeneous catalysts have been investigated for this reaction, each exhibits inherent drawbacks. In this work, we report the synthesis of $Ag/NiFe_2O_4$ magnetic nanoparticles as a highly efficient catalyst for the hydration of aromatic nitriles to primary amides. The physio-chemical properties of as-synthesized materials were established via various spectroscopic, microscopic, and physical techniques including FTIR, XPS, PXRD, EDS, FE-SEM, TEM, VSM, BET, and TGA. $Ag/NiFe_2O_4$ nanocomposite was found to be efficient for hydration of nitriles with up to 98% isolated yield. The catalyst was magnetically recoverable within a time span of 60 s and reusable up to the six catalytic cycles without any significant loss of catalytic activity. Excellent magnetic retrievability, superior recyclability and wider functional group tolerance and green solvent medium are the outstanding features of this protocol.

Keywords: Magnetic nanocomposite; Heterogeneous Catalysis; Primary amide; Hydration

Studies on the Effect of ZnS:Mn Nanoparticles on the Judd-Ofelt and Radiative Properties of Sm^{3+} Ions in a Sol-Gel Silica Matrix

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The study explores the spectroscopic behaviour of Sm^{3+} ions in Mn^{2+}-doped ZnS nanoparticles (ZnS:Mn NPs) co-doped silica matrix. The synthesis of pure ZnS nanoparticles (ZnS NPs) and Mn^{2+}-doped ZnS nanoparticles (ZnS:Mn NPs) were done using a simple chemical co-precipitation method. Production of ZnS crystals with average crystallite size 17 nm and spherical shaped NPs with sizes ranging from appx. 40-75 nm were confirmed by the X-ray diffraction (XRD) and Transmission Electron Microscopy (TEM) analysis. Sm^{3+} singly doped and Sm^{3+} co-doped samples were fabricated by incorporating these NPs with Sm^{3+} into a silica matrix via the sol-gel route, maintaining a constant Sm^{3+} concentration while varying the ZnS:Mn concentrations. The fabricated samples were characterized optically by using Ultraviolet- Visible (UV-Vis) absorption and photoluminescence (PL) measurements. The effect of ZnS:Mn NP concentration on the Judd-Ofelt parameters and the radiative properties of Sm^{3+} was evaluated. The notably higher Ω_2 value observed for this system suggests that ZnS:Mn NPs act as effective network modifiers. An increase in both absorption and PL efficiency was noted in the co-doped samples, attributed to the enhanced oscillator strengths of Sm^{3+} transitions as well as the energy transfer (ET) from the ZnS:Mn NPs. The PL behaviour showed significant concentration dependency of ZnS:Mn NPs and exhibited strongest emission at the 0.005 M ZnS:Mn concentration. The $^4G_{5/2} \rightarrow {}^6H_{9/2}$ emission transition of Sm^{3+}, which corresponds to the emission at 643 nm in the silica matrix, displayed improved radiative performance. These findings indicate that ZnS:Mn NPs co-doped with Sm^{3+} could be promising candidates for optoelectronic applications, such as lasers and light-emitting diodes (LEDs). Moreover, the concentration-dependent PL properties, along with the tunable optical characteristics, underscore the potential of these NPs for use in advanced photonic devices and sensors.

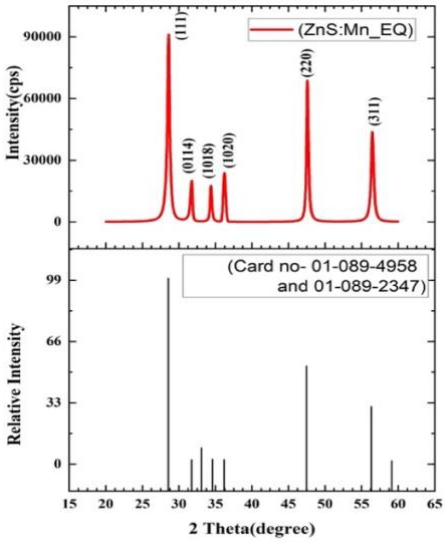

Figure 1: X-ray Diffraction for ZnS:Mn NPs with ICSD card

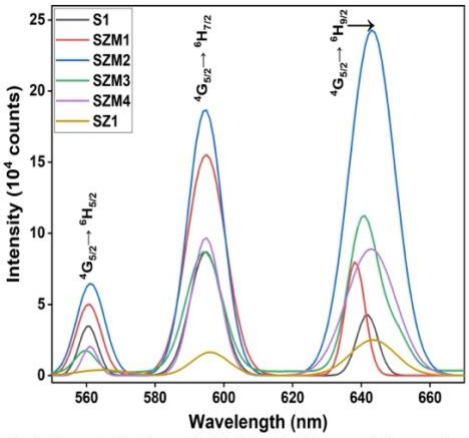

Fig. 2: PL spectra for the samples S1-SZ1 under 403 nm excitation wavelength.

Keywords: ZnS:Mn NPs; Silica matrices; Judd-Ofelt parameter; Radiative parameters

Fabrication of Lead-free Cu^{2+} doped $Cs_2AgBiCl_6$ Double Perovskite for Sustainable Photocatalysis

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The concept of multifunctional catalysts fuels the idea of sustainable development and environmental integrity. Lead-free Cu^{2+} doped $Cs_2AgBiCl_6$ (CABC X, X= mmol% of Cu dopant) double perovskite with an octahedral morphology has been developed and explored as a heterogeneous catalyst in the photo-reduction of nitroaromatics and photo-oxidation of benzyl alcohol. The synthesized CABC 30 sample efficiently catalyzed the nitrobenzene photo-reduction to aniline which is one of the most useful intermediate of pharmaceuticals, dyes, pigments, and pesticides and benzyl alcohol photo-oxidation to benzaldehyde, which serve as an important chemical component in the synthesis of vital perfume and cosmetic industry-related products [1-2]. The crystal phases of the synthesized materials were analyzed by PXRD analysis. In case of highly crystalline CABC, 2θ values at 23.39°, 33.30°, 41.10° and 47.78° are well-indexed to respective (220), (400), (422), and (440) crystal planes. The lattice constant decreases gradually on increasing the Cu-dopant from CABC to CABC 30. From SEM analysis, pure and doped CABC samples exhibit octahedral morphology. From in-depth PL measurements, CABC 30 is found to be the one with highest reduced recombination, which suggests better charge separation and enhanced photocatalytic activity. Following this, out of all composition, CABC 30 efficiently catalyze nitroaromatics photo-reduction and benzyl alcohol photo-oxidation under continuous irradiation of visible light with an excellent yield up to 99%.

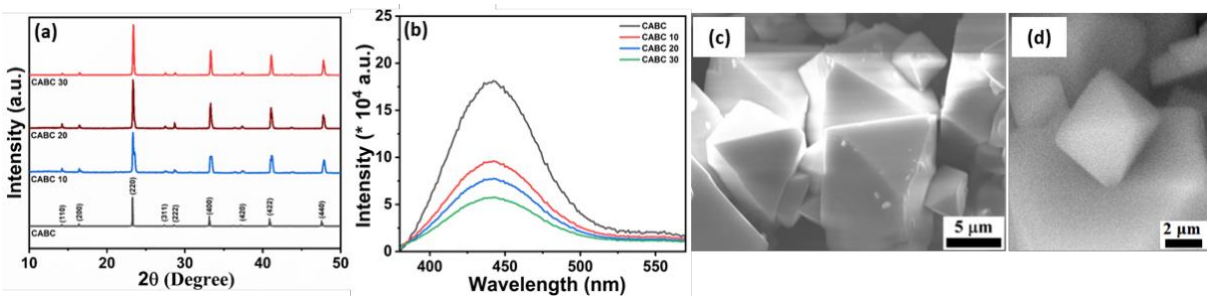

Figure: (a) PXRD, (b) emission spectra of pure and doped CABC samples, and (c), (d) SEM image of CABC 30

Keywords: Photocatalysis; Lead-free double perovskite; aniline; aromatic aldehyde

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Cluster Spin-glass Dynamics in Frustrated Trication Spinels

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Magnetically diluted compounds can be experimentally derived from conventional long-range ordered spinels like Co_3O_4 or Mn_3O_4 by elemental substitution at one or both of the cationic sites, tetrahedral (*A*) and octahedral (*B*), in the spinel lattice [1]. Such systems often provide an exciting platform to study magnetic frustration and random anisotropy leading to the loss of long-range magnetic order and emergence of exotic low-temperature phases like the spin-glass (SG) phase. In this work, we studied a doubly-diluted derivative of Mn_3O_4 exhibiting ferrimagnetic ordering, leading to a tri-cation spinel oxide: $ZnMnCoO_4$ (ZMCO). This system was synthesized using conventional solid-state synthesis techniques from binary transition metal oxides (ZnO, MnO_2, and Co_3O_4) as precursors. All of the *A*-sites in the 'parent' Mn_3O_4 lattice got replaced by nonmagnetic Zn^{2+}, while 50% of the *B*-sites got replaced by nonmagnetic Co^{3+} leaving the system with only one type of magnetic (Mn^{3+}) cations at the *B*-site.

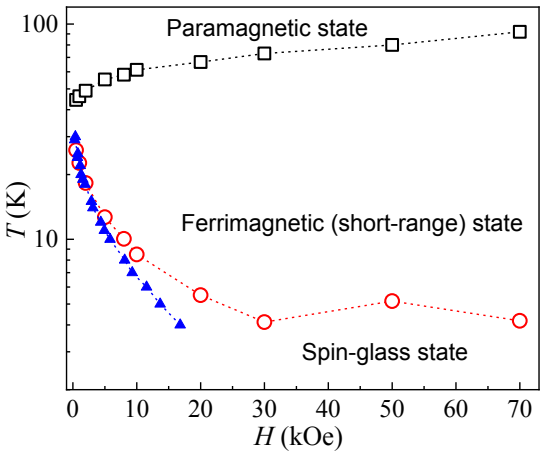

Fig 1. The phase diagram of ZMCO is mapped out on the *T*-*H* plane depicting the major phase transitions.

Polycrystalline ZMCO crystallized in cubic symmetry belonging to the space group *Fd*-3*m* as confirmed by x-ray diffraction. Although it appears quite simple, however, their nature of magnetism is complex and quite intriguing. Temperature and field dependent DC and ac magnetic measurements established a 'hierarchically organized' cluster SG ground state. This was further confirmed by a non-exponential time evolution of isothermal remanent magnetization. The presence of only short-range ordering in the investigated system was demonstrated by the absence of a λ-shaped peak in the specific heat versus temperature data [2]. Differential DC magnetic susceptibility plots revealed another transition in the system above the cluster SG phase. Above the 'glassy' transition, ZMCO exhibited ferrimagnetic behavior (T_{FN} = 38 K) with short-range magnetic correlations. A field-induced transition was also observed. All these are represented on the *T*-*H* plane as shown in Fig. 1. Thus, magnetically diluted spinels provide valuable insights on the frustration driven spin dynamics in complex oxides, affected by the role of elemental substitution.

Keywords: Spinel oxides, Magnetic Frustration, Spin-glass.

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Investigation on the Correlation of Optical Parameters of Nanocrystalline ZnS_xSe_{1-x} thin Films with Deposition Temperature

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Ternary ZnS_xSe_{1-x} thin films were deposited on glass substrates by a soft, cost-effective chemical bath deposition (CBD) technique at different deposition temperatures. The effect of the deposition temperature on the optical properties of the films was studied using UV-visible spectroscopy. The optical transmission graph revealed that all the films have 70-80% transmittance in the visible range, and the transmittance decreases with the increase in deposition temperature. The absorption and reflection of the films were found to increase with deposition temperature. The optical energy band gap was calculated using Tauc's plot, and it was found to decrease with the increasing deposition temperature. The observed optical properties of the ZnSSe thin films prove their potential to be used as a window layer for solar cells and other optoelectronic applications.

Keywords: ZnSSe; thin films; optical properties; Chemical bath deposition

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Modulation of the Structure and Dielectric Properties of $ErCrO_3$ by Introducing Fe^{3+}

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Polycrystalline samples of $ErCr_{1-x}Fe_xO_3$ (x = 0.00, 0.05, 0.10 & 0.15) were prepared by using sol-gel technique in single phase form. The obtained XRD patterns were Rietveld refined using FullProf software and result of refinement revealed the expansion of unit cell upon substitution of Fe^{3+} ion on Cr^{3+} site due to its higher ionic radii than Cr^{3+}. Different characterization techniques such as Scanning Electron Microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDX) and Raman Spectroscopy were employed to study the crystal structure, surface morphology, chemical composition and bonding information of the composed samples. The dielectric characteristics of the samples were determined by analyzing the impedance spectroscopy data. Analysis of the impedance data (Z' and Z'') revealed a discontinuity in the resistive behavior for all the samples suggesting the appearance of positive temperature coefficient of resistance (PTCR) like region over a wide range of temperatures. Study of dielectric constant and AC conductivity data corroborated the similar trend. In addition, all the $ErCr_{1-x}Fe_xO_3$ samples showed colossal value of dielectric constant (>10^4) at room temperature, supporting their potential use in electronic devices. The AC conductivity data of the samples were analyzed using Jonscher Power Law (JPL) which suggested the existence of two mechanisms in the conduction process: Correlated Barrier Hopping (CBH) and Small Polaron Hopping (SPH).

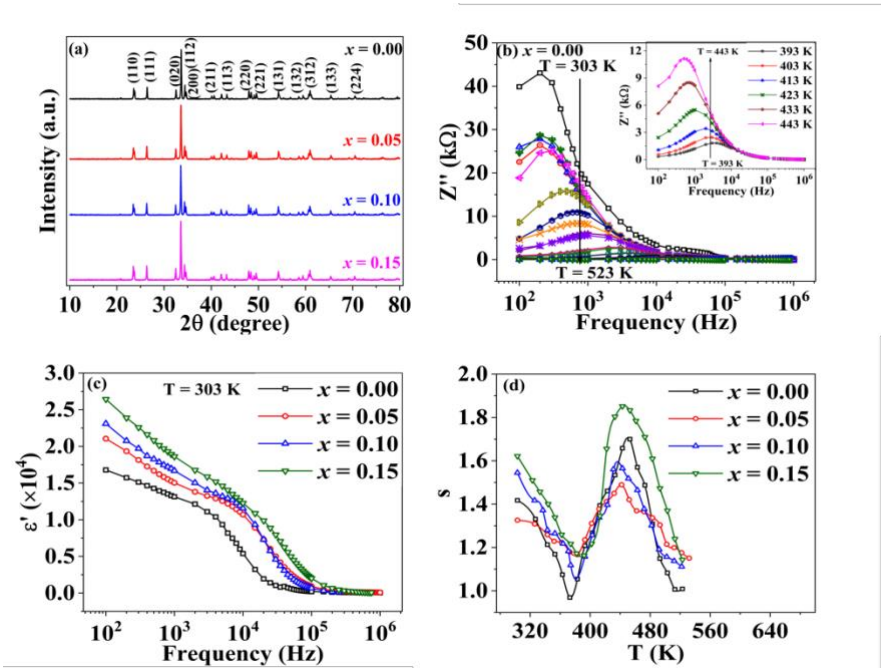

Fig. 1: (a) Room temperature XRD patterns, (b) Z'' vs f for x = 0.00, (c) ε' vs f for all samples, (d) Frequency exponent (s) vs. T for all samples

Keywords: Orthochromites; Perovskites; Sol-gel process; Impedance spectroscopy

Investigating the Impact of Cr Substitute in $BaNi_2Fe_{16}O_{27}$ W-type Hexaferrites on its Structure, Electrical and Magnetic Properties for Microwave Absorber

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In this work, substitution of Cr^{3+} in W-type Hexaferrites (WHF) i.e., $BaNi_2Fe_{16-x}Cr_xO_{27}$ (x=3%, 5%, 7%) was tuned for its various applications in the fields of microwave absorber. Cr^{3+} was substituted in Fe^{3+} using sol gel self-auto combustion chemical reaction annealed at 900°C for 5 hrs. The effect of Cr^{3+} on WHF was analyse by XRD and Rietveld refinement shows the present of WHF with space group of $P6_3/mmc$ with secondary phases of $BaFe_{12}O_{19}$ (MHF) and α-Fe_2O_3 (hematite), decreases in average crystallite size from 24 nm to 13 nm, structural changes and sites occupies by Cr^{3+} in WHF was observed. The dielectric (ε', ε''), magnetic (μ', μ'') and reflection loss at various frequency of X-band was study for microwave absorption.

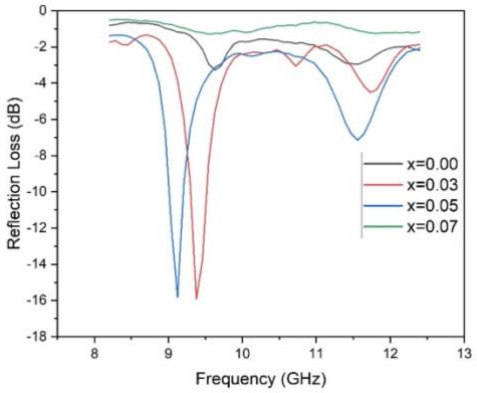

Fig. 1: Reflection loss of $BaNi_2Fe_{16-x}Cr_xO_{27}$ (x=3%, 5%, 7%).

Keywords: XRD; Rietveld refinement; microwave absorber.

References:

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Modelling of Homo- and Hetero-structures based on MgS and MgSe Monolayers

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Two-dimensional homo-and hetero-structures based on alkaline earth metal chalcogenide monoplanar monolayers (ML) are found to have promising mechanical, electronic, optical and thermal properties[1,2]. We have studied the structural and electronic properties of alkaline earth metal based chalcogenide ML such as MgS and MgSe. Moreover, different homo- and hetero-structures of these MLs have been investigated by increasing the number of layers to form bi- (BL), tri- (TL) and tetra-layer (TtL) systems. Accordingly, MgS-MgS, MgSe-MgSe, MgS-MgSe (BLs); MgS-MgS-MgS, MgSe-MgSe-MgSe, MgS-MgS-MgSe, MgS-MgSe-MgS, MgSe-MgS-MgSe, MgSe-MgSe-MgS (TLs); MgS-MgS-MgS-MgS, MgSe-MgSe-MgSe-MgSe, MgS-MgS-MgSe-MgSe, MgS-MgSe-MgSe-MgS, MgSe-MgS-MgS-MgSe, MgSe-MgS-MgSe-MgS (TtLs) have been modelled using DFT code of the Quantum ESPRESSO package. The configuration of the multi-layered structures is chosen in such a way that their constituent monolayers follow the similar orientation. All of these structures are be found to planar. Based on the computed binding energy, we can say that, all systems are structurally stable . All the 2D systems are semiconductors having indirect electronic energy band gap (E_g) and they are non-magnetic in nature. E_g gets successively reduced if we increase the number of layers up to three for homo-structures of both MgS and MgSe. In contrast to this, the band gap of TtL homo-structures of MgS is same as its TL homo-structure, but for TtL MgSe hetero-structure the bandgap is equal to the BL MgSe homo-structure. The multi-layered hetero-structures exhibit lower E_g values than their constituting monolayers. Therefore, modelling of homo- and hetero-structures based on MgS and MgSe MLs plays an important role in tuning the electronic properties of the systems.

Keywords: monolayers, homo-structure, hetero-structure, electronic properties

References:

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Solvent treated Dielectric Properties and Characterisation of TiO_2 nanoparticles

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Titanium dioxide nanoparticles (TiO_2 NPs) were green synthesized with solvent alteration, using DI water and ethanol as solvents. During green synthesis, Nyctanthes Arbor-Tristis (Night Jasmine) and Azadirachta Indica (Neem) leaf extract were used as reducing agent. The influence of these solvents on the morphological and structural properties of the TiO_2 nanoparticles was systematically studied using Field Emission Scanning Electron Microscopy (FESEM), and UV-Visible (UV-Vis) spectroscopy. FESEM analysis revealed distinct morphological variations in nanoparticle size and shape depending on the solvent used. As far as dielectric properties of TiO_2 NPs are concerned, they are assessed via VNA (Vector Network Analyser). The variation in permittivity and permeability hints at solvent treated dielectric properties. This study highlights the significant role of solvent alteration in tailoring the dielectric properties, loss tangent measurement of TiO_2 nanoparticles for potential applications in microwave absorption, photocatalysis and environmental remediation.

Keywords: TiO_2 NPs; Solvent; Permittivity; Permeability

Studies on Annealing Effect on Structural Properties of Pristine and Copper-Doped Iron Oxide Nanoparticles

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In this present work, pristine and Copper (Cu) doped iron oxide thin films were deposited on a glass substrate by the Reactive Vapour Plasma Mixing method. The thin films were deposited at a substrate temperature (S_T) of 400 °C in a vacuum chamber with a base pressure of approximately 8.6×10^{-6} mbar. The films were annealed for 1 hour at an annealing temperature (A_T) of 400 °C in a background pressure of ~ 10^{-6} mbar. The effect of annealing temperature on the crystal structural properties of iron oxide nanoparticles was investigated by X-ray Diffraction (XRD) analysis. The XRD results revealed the formation of Fe_2O_3 and Fe_3O_4 nanoparticles. The progressive increase in intensity of the Cu-doped sample in comparison to the pristine sample was observed. The average crystallite size of the nanoparticles was calculated using the Scherrer formula. The crystallinity of the annealed film was better in comparison to as deposited sample. The annealing temperature played an important role in the formation of better crystalline nature of the iron oxide nanoparticles.

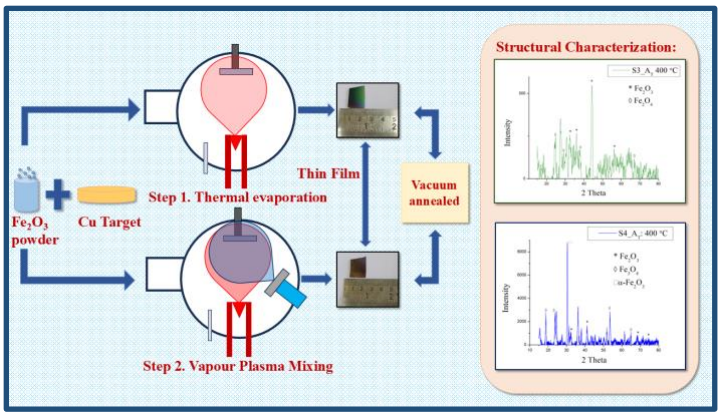

Fig. 1: Graphical abstract.

Keywords: pristine; plasma; vacuum; iron oxide nanoparticles.

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Antisite Defect Tuned $NaEu(WO_4)_2$ Material: an Efficient Red Phosphor for Optoelectronic Applications

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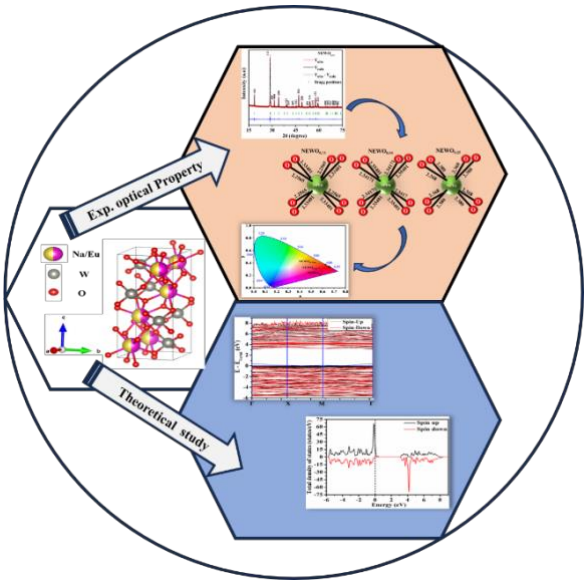
Sodium europium double tungstate ($NaEu(WO_4)_2$) material has been synthesized at different amount of trisodium citrate (Na_3cit) assisted hydrothermal technique, followed by calcination to promote crystallinity and detail investigations on their crystal structures, luminescence properties. The structural evolution of our samples has been studied by x-ray diffraction, Rietveld refinement, Fourier transform infrared and Raman spectroscopies. $NaEu(WO_4)_2$ belongs to scheelite family with Na, Eu atoms occupying same sites, as well as $Eu_{Na}^{m\bullet}$ antisite defects deforming EuO_8 dodecahedra. We have found out modulation of W – O, Eu – O and angle splitting in the presence of $Eu_{Na}^{m\bullet}$ antisite defect. From in depth x-ray photoelectron spectroscopy, we have validated deformation of EuO_8 dodecahedron due to presence of oxygen vacancy (V_O), originated from $Eu_{Na}^{m\bullet}$ antisite defect. Herein, we have shown that band gap of $NaEu(WO_4)_2$ is highly sensitive to defects. However, the intense $^5D_0$-$^7F_2$ transition of Eu^{3+} at 615 nm with CIE color coordinate (0.67, 0.33) is very prominent to make $NaEu(WO_4)_2$ suitable red phosphor material for near UV type light emitting devices (LEDs). Furthermore, to validate our experimental observations theoretically, we have calculated band structure and density of states of $Eu_{Na}^{m\bullet}$ antisite defect containing $NaEu(WO_4)_2$ using *ab initio* density functional theory.



Schematic: Eu-O bond length distortion modified red emission and theoretical model study of $NaEu(WO_4)_2$ material

Keywords: Scheelite type material, antisite-defect, luminescence, ab initio density functional theory

Exploring of Reduced Graphene Oxide (rGO) Composite Materials for Advancement in Biomedical Applications: A Comprehensive Review

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Composites utilizing reduced graphene oxide (rGO) have attracted significant research interest, mainly due to its outstanding physical, chemical, electrical, mechanical, thermal and optical properties. There are several applications for rGO and its composites across various sectors, including sensing, battery enhancement, photocatalysis, supercapacitors and biomedical uses. This comprehensive analysis investigates reduced graphene oxide (rGO) and its different composites in the biomedical sector. Our research review indicates that rGO is an exceptionally versatile material that can effectively merge with different components, making it suitable for a variety of medical applications and open up new pathways for future medical advancements. We focus on the fundamental properties of rGO, such as its compatibility with living beings, excellent electrical conductivity and substantial surface area, which enhance its effectiveness. By analyzing findings from multiple research efforts, we illustrate how rGO-based composites play a vital role in developing innovative materials and solutions in the biomedical field.

In this review we explored rGO composites sensor detecting a variety of chemical and biological targets. The review included H1N1 virus, HTLV-1, cancer cells (e.g., HELA, MCF-7) and biomolecules such as H-IgG, glucose, L-arginine, and the N-protein of SARS-CoV-2 etc. We also examined their use in detecting small molecules like chloramphenicol (CAP), paracetamol (PAR), methanol and caffeine, as well as chloride ions and ascorbic acid (AA), dopamine (DA) and Uric acid (UA). Additionally, complex analytes like methylene blue (MB) and low-density lipoprotein (LDL) were reviewed. This comprehensive review emphasizes the significant potential of rGO in material science for healthcare applications.

Keywords: reduced graphene oxide (rGO); composites; biomaterials

Sustainable pH Indicator Using Natural Flavonols from Onion (Allium cepa) Husk

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The growing interest in environment friendly and cost-effective pH indicators has driven the exploration of natural compounds with desirable properties. In this study, we report the successful extraction of natural Flavonols from onion (Allium cepa) husk using ultrasound-assisted extraction, presenting a sustainable alternative for pH sensing applications. The extract was characterized using Fourier transform infrared (FTIR) spectroscopy, ultraviolet-visible (UV-Vis) absorption spectroscopy, proton nuclear magnetic resonance (^{1}H NMR) and Fluorescence (PL) spectroscopy. The FTIR spectrum clearly identified key vibrational modes in the extract, including hydroxyl groups (3380 cm^{-1}) and carbonyl groups (1655 cm^{-1}), indicative of flavonol structure. The UV-Vis Spectroscopic analysis revealed characteristic flavonol absorption bands at 263 nm, 297 nm and 367 nm. ^{1}H NMR confirmed the presence of hydroxyl groups at the 3-OH and 5-OH positions, key sites in the flavonol structure. PL measurements further validated flavonol's spectral features with distinct emission peaks. The concentration of flavonol was estimated to be 2.59 mg RE/g of dry onion husk by using an aluminum chloride colorimetric method, with rutin as the standard flavonol. The pH sensing study was performed by both UV-Vis absorption and PL emission spectroscopy under varied pH conditions by adding NaoH or HCL. The colour of the extract changed from pink in acidic conditions to light yellow and dark brown in basic conditions. The absorption spectra exhibited significant spectral shifts corresponding to colour changes of the extract. A linear dependence on pH was observed in acidic media, described by the equation $y = 1.3987x + 0.0287$ with an R^2 value of 0.97. Additionally, the fluorescence spectra showed a linear increase in intensity with increasing pH, described by the equation $y = 37445x + 19892$ and an R^2 value of 0.99. These changes were attributed to protonation and structural modifications of the flavonol molecules. This study highlights the promising role of onion-derived flavonols as natural, sustainable pH indicators, offering an eco-friendly solution for applications in analytical chemistry, environmental monitoring and beyond.

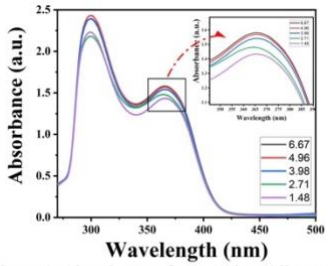

Figure 1: Absorbance of extract in acidic medium.

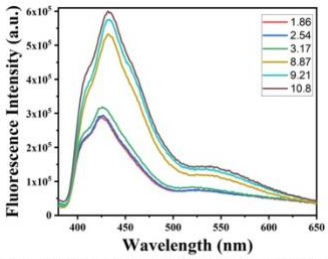

Figure 2: Fluorescence of extract in different pH.

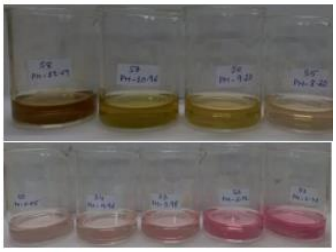

Figure 3: Colour of extract in different pH.

Keywords: Sensing; pH indicator; Onion husk; Sustainable

Synthesis of CdSe Nanoparticles in Aqueous Medium

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Research in nanoscience and nanotechnology is expanding in different fields including physics, chemistry, biology, engineering, medicine etc. because of it's fascinating and noble properties. Nanoparticles can be synthesized in various method. We have followed chemical bath deposition (CBD) method for the purpose of synthesis. Nanoparticles are unstable in nature, because of presence of large number of anion, cation and free radicals on their surface. This leads to agglomeration of nanoparticles into larger particles. Capping of nanoparticles with organic ligands or long chain organic molecule can provide stability to the nanoparticles under ambient condition. We have synthesized stable spherical CdSe nanoparticles in aqueous medium in a single pot chemical reaction with L-cysteine organic ligand capping. We have studied the structural and optical properties of the nanoparticles by spectroscopic, scattering and microscopic analysis. The UV Visible spectroscopy is recorded which gives the idea of band gap energy. The X-Ray Diffraction (XRD) confirms the crystalline nature of the nanoparticles. The transmission electron microscopy (TEM) gives the precise information about the nanoparticles size and shape. The size of the nanoparticle is found to be 8nm from the TEM micrographs. The size estimated from the X-Rady diffraction are in good agreement with the TEM results.

Eco-Friendly Ag-Nanoparticles as Corrosion Inhibitors for Mild Steel

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Corrosion of mild steel poses significant economic and environmental challenges across various industries. Recently, there has been growing interest in the use of environmentally friendly corrosion inhibitors, particularly Ag-nanoparticles derived using plant extracts. Ag-nanoparticles exhibit exceptional inhibitory characteristics due to their eco-friendly nature and ability to form a protective barrier on the metal surface, thereby retarding the corrosion process. Further, the green synthesis of Ag-nanoparticles using plant extracts has emerged as a simple, cost-effective, and environment-friendly approach that mitigates the involvement of toxic chemicals. Thus, this paper provides a panoramic analysis of the diverse techniques employed in the synthesis of Ag-nanoparticles using plant-based sources, and explores the potential of these AgNPs as effective corrosion inhibitors for mild steel. Moreover, it investigates the mechanisms of corrosion inhibition, inhibitory efficiencies, and the latest developments in this field. It also discusses the challenges and potential opportunities in utilizing plant-derived AgNPs as eco-friendly corrosion inhibitors for mild steel, with the aim of providing guidance for further research and development in this field.

Keywords: Plant extract; Silver Nanoparticles; Mild Steel; Corrosion Inhibitor

References:

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One Step Hydrothermally Synthesized Ruthenium Doped Molybdenum Disulfide: towards High-performance Symmetric Supercapacitor Device Application

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The limited availability of fossil fuels, along with their high cost, consumption, and substantial environmental effects, drives the need for developing sustainable clean energy solutions. Molybdenum-based electrode materials are recognized for their excellent energy storage stability, high energy, and power density, making them effective choices for improving the performance of energy storage devices. Here, ruthenium (Ru) doped molybdenum di-sulfides (MoS_2) are successfully synthesized by cost-effective one-step hydrothermal methods with various Ru doping percentages (2%, 5%, and 10%). Among the different Ru doping contents, the prepared compound with 5% Ru shows a very good electrochemical performance with maximum capacitive performance. The specific capacitance of this compound is found to be 489 F g^{-1} at a scan rate of 1 mV s^{-1} from cyclic voltammetry (CV) and 287 F g^{-1} at a specific current 1 A g^{-1} from galvanostatic charge-discharge (GCD) measurements whereas the pure MoS_2 exhibits specific capacitance 324 F g^{-1} and 125 F g^{-1} respectively under the identical condition. The symmetric super-capacitor device fabricated with 5% ruthenium doped MoS_2 demonstrates wider working potential window 2 V, higher energy density of 42 Wh kg^{-1} at a specific current 1 $Ag^{-1,}$ and noticeable power density of 8 kW kg^{-1} at a specific current of 10 A g^{-1}. A prolonged cycling stability of 99.71% retention of specific capacitance over 5000 GCD cycles in 5% ruthenium-doped MoS_2 is achieved compared to the pure MoS_2 with 30% retention over the same number of GCD cycles. This is expected due to the proper incorporation of Ru atoms into the Mo sites. The EIS spectra reveal this compound's lowest charge transfer and solution resistance, which suggests its higher conductivity. The outstanding performance of the 5% ruthenium-doped MoS_2 electrode compound indicates its great potential for applications in high-performance energy storage systems.

Keywords: Simple hydrothermal synthesis, Supercapacitor applications, Wide potential window, Excellent stability

Impact of pH on the Structural Properties of Chemically Deposited $Zn_xMg_{1-x}S$ Thin Films for Photovoltaics

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This study reports on the growth and structural characterization of nanocrystalline $Zn_xMg_{1-x}S$ (ZMS) thin films, which are being investigated for optoelectronic applications such as photovoltaic cells. The research examines the effect of pH on the structural properties of the thin films, focusing on how changes in pH influence these properties. ZnMgS, a wide-bandgap semiconductor, has shown alterations in its structural characteristics due to variations in pH. The primary objective of this analysis is to investigate the structural characteristics of the ZnMgS thin films, with a focus on their suitability as window layers in solar cells. X-ray diffraction studies revealed that the as-prepared films are nanocrystalline and possess a cubic phase with a preferred orientation along the (111) plane. With the increase in pH values, the peak positions shifted to the higher 2θ values and the intensity increased. X-ray diffraction (XRD) is used to determine several important parameters, including lattice constant, crystallite size, dislocation density, and microstrain. The results highlight the promising structural properties of ZnMgS thin films, underscoring their potential in the fabrication of optoelectronic devices, particularly in enhancing the efficiency of solar cells.

Keywords: Thin film, Photovoltaics, Structural properties, X-ray diffraction

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Kalanchoe pinnata Leaf Extract-assisted Green Synthesis of Fe_3O_4-rGO Doped PTh Nanocomposite for Highly Sensitive Room Temperature Chloroform Gas Sensor

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Chloroform ($CHCl_3$ - Trichloromethane) is a chlorinated volatile organic compound (Cl-VOC) with well-documented toxicity and carcinogenic effects. Herein, we report a successful synthesis of highly conductive polythiophene-magnetite-reduced graphene oxide nanocomposite (PTh-Fe_3O_4-rGO) for enhanced Chloroform gas sensing application in room temperature. The PTh-Fe_3O_4-rGO nanocomposite was synthesized by in-situ polymerization method using a novel and cost-effective process. The prepared material was characterized by different techniques such as powder x-ray diffraction, field emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM), Fourier transform infrared (FTIR) spectroscopy, BET and UV-Vis spectroscopy. The nanocomposite PTh-Fe_3O_4-rGO has showed enhanced Chloroform vapour sensing performance characteristics compared to rGO-Fe_3O_4 and pure Fe_3O_4 which have been reported earlier. The nanocomposite provide improved sensitivity mainly due to a high surface area (49 m^2/ g) with doping of PTh by rGO and Fe_3O_4. The nanocomposite also show excellent electrical and electrochemical properties with a faster response and recovery time across different concentrations (10, 50 and 100 ppm) due to high diffusivity of vapours into the structure owing to the 3-Dimensional nature of the nanocomposite structure which makes the directly exposed area multifolds.

Keywords: Chloroform; polythiophene; reduced graphene oxide; green synthesis

Studies on Microstructural Properties of Chemically Synthesized MgO Nanocrystals

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In this study, pure magnesium oxide (MgO) nanocrystals were synthesized using the chemical co-precipitation method. The Scherrer's formula was initially used to estimate the crystallite size, which gave a value of 11 nm. The microstructural properties of the MgO nanocrystals were further analyzed using different formulations of the Williamson-Hall (WH) method of X-ray diffraction line profile analysis. The WH analysis was carried out using three different models viz. uniform deformation model (UDM), uniform stress deformation model (USDM) and uniform deformation energy density model (UDEDM). The crystallite size (D) obtained from the UDM was 13±1 nm, while both the USDM and UDEDM yielded a crystallite size of 14±1 nm. In addition to the crystallite size, the strain (ε), stress (σ) and energy density (u) of the MgO nanocrystals were determined through the WH analysis. The strain, stress and energy density were found to be $(7.6\pm3.5)\times10^{-4}$, (379±112) MPa and (165±117) kJm^{-3}, respectively. Optically, MgO is a direct band gap semiconductor material. The band gap energy was determined from the UV-visible absorption spectra using the Tauc's plot, which gave a value of 4.70 eV. In conclusion, the preliminary investigation shows that a simple chemical method can be used to obtain MgO nanocrystals with minimal internal stress and strain. Further, the nanocrystals exhibited a wide band gap of 4.70 eV, which makes it a favorable material for application in areas like photocatalysis.

Keywords: MgO nanostructure; Williamson-Hall method; Microstructure; Band gap

Boosting the Piezoresponse in Ferroelectric Polymer via Perovskite Nanoparticle Incorporation

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Owing to their superior flexibility, high stability, easy processibility, low cost and lightweight nature, ferroelectric polymers are considered as a versatile and ideal option for the development of advanced flexible and wearable electronic devices. Their ability to produce electrical energy from applied stress, probably reducing the need for external power sources. In this work, we have synthesized poly(vinylidene fluoride) (PVDF) polymer and $CsPbBr_2I$ perovskite nanocomposite. The structural, morphological and compositional details of the $CsPbBr_2I$ nanorods, synthesized by ligand assisted reprecipitation method are thoroughly investigated through XRD, FESEM and EDS analysis. The influence of $CsPbBr_2I$ nanorods on the piezoelectric property of PVDF has also been explored via XRD and FTIR analysis of the nanocomposites. FTIR analysis reveals that 0.5 wt% loading of $CsPbBr_2I$ in PVDF matrix leads to an 87% activation in electroactive phase content, as a consequence of interfacial interaction between PVDF molecular dipole and $CsPbBr_2I$. The fabricated piezoelectric nanogenerator (PENG) with optimized concentration (0.5%) of $CsPbBr_2I$ achieves an open circuit voltage of 6.22V which is 3 times higher than its pristine counterpart.

Keywords: Nanogenerator, Perovskite, Nanocomposite

JQ1 and Doxorubicin loaded Prussian Blue based Nanoplatform for Immunotherapeutic Treatment against Triple Negative Breast Cancer

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Triple-negative breast cancer (TNBC) constitutes 10–20% of breast cancers and is challenging to treat due to a lack of effective targeted therapies. At present, surgical resection, chemotherapy, and radiotherapy have been the three main treatments for cancer, while poor efficiency and obvious side effects limit their clinical application. To address these challenges we have tried to develop nanocomposite based targeted drug delivery, which has fulfilled therapeutic as well as diagnostic clinical strategies. Two anticancer drugs (JQ1 and Doxorubicin) have been incorporated on NIR active prussian blue nanocube (PBNC) which have been engineered to make biocompatible and target specific drug carrier. This nanoplatform has been addressed to accomplish inhibition of proliferation marker (e.g.: KI-67), program cell death 1 (PD-1) and program cell death ligand 1 (PD-L1) and occur pyroptotic cell death in *in-vitro* model. Taken together, our study demonstrates a compact and simple nanoplatform for multiple therapy like targeted therapy, photo dynamic and thermal therapy (PDT & PTT), and immunotherapy, for TNBC treatment and also fulfil better MRI contrast efficacy as its diagnostic potentiality.

Keywords: JQ1, Antiproliferation, Pyroptosis, Immunotherapy

Eco-Friendly Synthesis of $NiFe_2O_4$ Nanomaterials: A Green Approach to Advanced Catalysis for Enhanced Oxidation of Benzyl Alcohol

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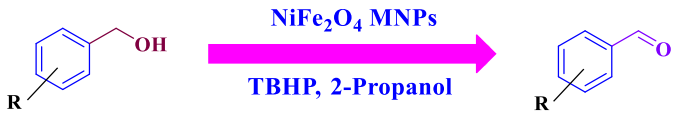
Nickel ferrite ($NiFe_2O_4$) nanomaterials have gained widespread attention as a promising class of materials, renowned for their unique magnetic, catalytic, and structural attributes. This study presents an environmentally sustainable method for synthesizing $NiFe_2O_4$ magnetic nanomaterials, utilizing *Camellia sinensis* var. Assamica (tea) leaf extracts. The nanomaterials' physico-chemical properties were determined through various advanced techniques, including SEM-EDX, VSM, XPS, TEM, and powder diffraction XRD. Remarkably, the synthesized $NiFe_2O_4$ nanomaterials exhibit exceptional catalytic efficiency, especially in the oxidation of benzyl alcohol, establishing them as a valuable asset in green chemistry applications. The synthesized nanomaterial as catalyst can be readily separated from the reaction mixture using a magnet and maintain their catalytic activity consistently for up to five catalytic cycles without significant loss of its activity. This oxidation process is essential for producing benzaldehyde, a crucial compound utilized in the production of fragrances and pharmaceuticals. Moreover, it offers a selective route for converting alcohols into aldehydes, thereby enhancing the efficiency of synthetic pathways in organic chemistry.



Scheme: Oxidation of various benzyl alcohols catalyzed by $NiFe_2O_4$ nanomaterials.

Keywords: Nanomaterials; Nickel ferrite; Magnetic nanoparticles; Heterogenous catalysis

Small *in situ* Generated Ligand based Highly Conductive Metal Organic Frameworks

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Four isostructural formate based electrically conductive metal organic frameworks namely, $[H_2N(CH_3)_2][M(HCO_2)_3]$ (M=Mn; **Mn-F**, M=Co; **Co-F**, M=Ni; **Ni-F**, M=Zn; **Zn-F**), were synthesized with simple and cost effective methods. The *in situ* generated formate ion was attributed to decomposition of DMF, which was used as solvent of the reactions, under high pressure and temperature. Single crystal X-ray diffraction analysis reveals that MOFs also contain *in-situ* generated dimethyl ammonium cation inside their pores to maintain the charge neutrality of the framework. As-synthesized MOFs exhibit impressive room temperature electrical conductivity considering the electrical conductivity of MOFs reported so far. All the MOFs are semiconducting in nature and their conductivities increases with temperature. Again, Upon removal of guest from the pores the room temperature electrical conductivity of all the frameworks were improved except for **Co-F**. The theoretical evaluation of band of the MOFs reveals that through bond conductivity is siganificantly determined by the number of high spin electron in the metal d-orbitals.

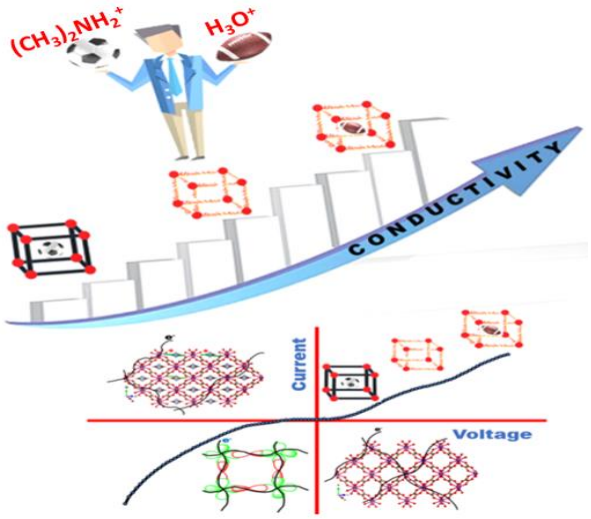

Fig. 1: Graphical representation of the work.

Keywords: Band gap; conductivity; *in situ*; Metal-organic framework

Surface Modification of $BaTiO_3$-based Perovskite Nanocrystals for High Energy Storage Applications

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Barium titanate ($BaTiO_3$) nanoparticles (BTNPs) have gained attention over the past few decades, because of their excellent qualities such as dielectric and piezoelectric topologies, and dielectric and optical capabilities. In this study, $BaTiO_3$ nanocrystals were synthesized using the co-precipitation method. The process was optimized by adjusting parameters such as temperature, and pH to achieve a uniform particle size distribution. The synthesized $BaTiO_3$ nanocrystals were characterized by X-ray diffraction (XRD), UV-visible spectroscopy, Scanning electron microscopy (SEM) and Transmission electron microscopy (TEM) to determine their crystallinity, optical property, morphology, and particle size. Uniform and agglomerated, cubical shaped particles of <100 nm are observed by scanning electron microscopy (SEM). Moreover, the TEM image of as prepared $BaTiO_3$ power confirmed the formation of cubical nanoparticles (~40 nm) XRD pattern of $BaTiO_3$ nanoparticles that width is (~15.95 nm) in the (110) orientation. The optical property of as prepared $BaTiO_3$ has studied by UV-visible absorption spectra. A sharp peak of absorption is observed around 302 nm corresponding to characteristic optical bandgap and gradually falls to became minimum. The estimated direct bandgap from Tauc plot is found to be around 3.14 eV. The optimized sample will be tested for energy storage application in MIM (metal-insulator-metal) structure.

Keywords: Perovskites, energy storage, nanoparticles, bandgap

Fabrication of PVDF-CuO Membrane for Oily Wastewater Treatment

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In this study, we fabricated polyvinylidene fluoride (PVDF) membranes through electrospinning and enhanced them by growing copper oxide (CuO) nanostructures using a hydrothermal process. The goal was to explore the potential of this PVDF-CuO composite membrane for effective oil-water separation and photocatalysis. By combining the structural flexibility of PVDF with the catalytic properties of CuO, the membrane was designed to separate oil from water while also breaking down organic pollutants under light exposure. This work opens up possibilities for advanced applications in environmental water treatment, addressing both separation and degradation challenges.

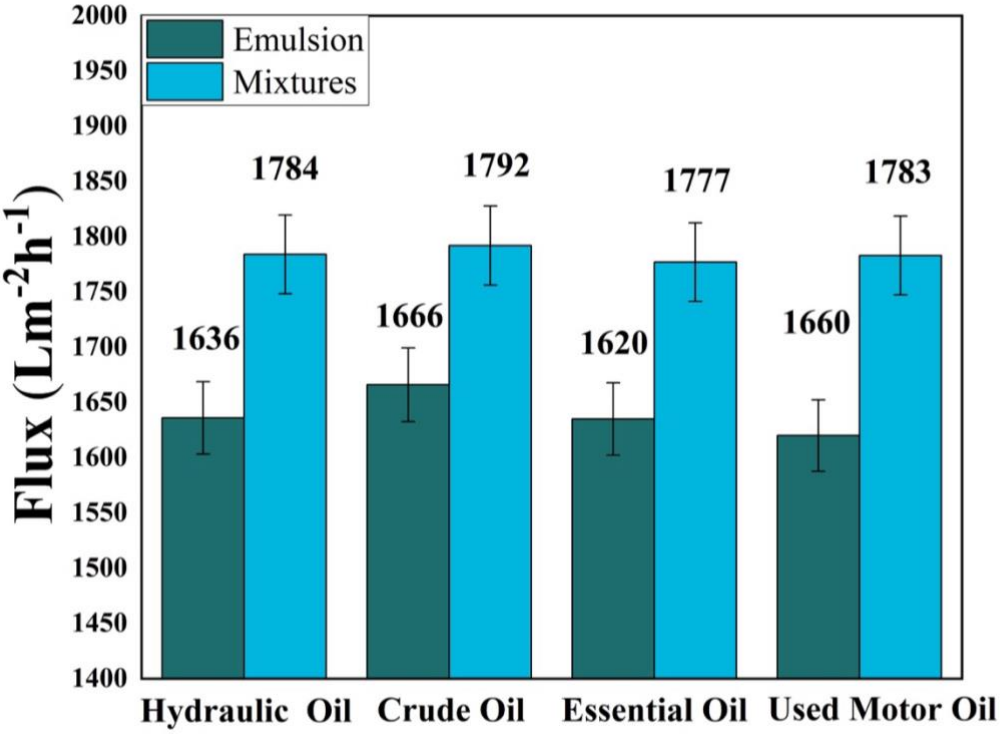

Fig. 1: Flux of oil-water separation for various oil Mixtures and Emulsion (Used Motor Oil, Essential Oil, Crude Oil and Hydraulic Oil)

Keywords: PVDF; CuO; Photocatalysis; Oil-water separation


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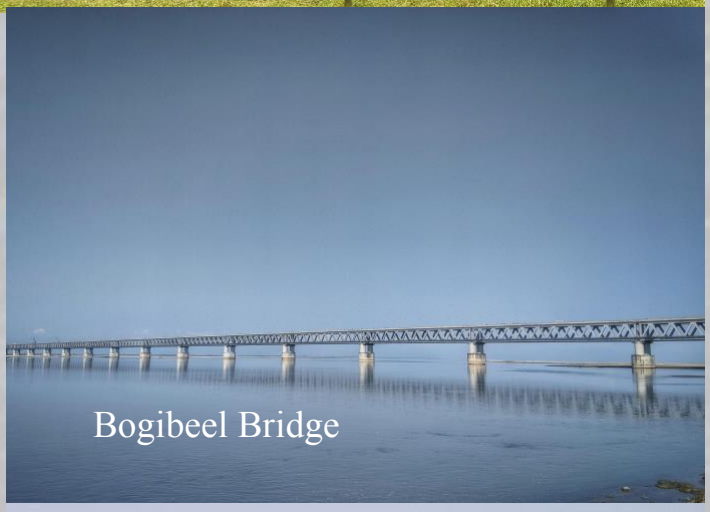
Bogibeel Bridge


Dibru Saikhowa National Park


Rangghar, Sivasagar