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ABSTRACTS

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4th National Conference on
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64	Synthesis, single crystal growth and characterization of a new Chalcone	Sandhya[a] Ravindra H.J[a] R Puranik H[a,b] Vijaya Kumari[a,c] Vinayak Bhat[a] S.M. Dharmaprakash[d]	[a] Department of Physics, Shri Madhwa Vadiraja Institute of Technology and Management, Bantakal, Udupi-574115 [b] Department of Physics, Dr. G. Shankar Government Women's First Grade College, Ajjarkadu, Udupi-576101 [c] Department of Physics, Sri Bhuvanendra College, Karkala-574199 [d] Department of Physics, Mangalore University, Mangalagangotri, Karnataka, 574199, India
65	Structural and optical properties of Curcumin- PVA-ZnO composite nano thin films deposited by RF magnetron sputtering	Jyothi Soudi[a] Vinoditha U[a] K M Balakrishna[a] B K Sarojini[b]	[a] Department of Physics, Mangalore University,Magalagangothri,-574199, Mangaluru, Karnataka, India [b] Department of Industrial Chemistry, Mangalore University, Magalagangothri,-574199, Mangaluru, Karnataka, India

IT-01

Advances in Supercapacitor Materials and Technology

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ABSTRACT

The advancement in modern society needs an efficient, sustainable and environment friendly energy harvesting and storage device. Supercapacitor is a charge storage device that provides high energy storage capacity, fast charge or discharge and long cycle life. It stores energy in the form of electrical double layer or by fast surface redox reactions. It complements or replaces battery in electrical energy storage applications during pulse power requirement. It is being used in hybrid electric vehicles and static energy storage, consumer electronics as well as many defence applications. Different physical forms of carbon having high specific surface area exhibit double layer type capacitance and long cycle life. Transition metal oxides, conducting polymers and their composites are being exploited as the electrode materials. The metal oxide and conducting polymer based electrodes work on redox processes and hence exhibit higher specific capacitance but limited cycle life. Aqueous, non-aqueous and solid polymer based electrolyte finds applications in supercapacitor. However fabrication of actual device is an involved process.

Even though supercapacitor is being used, the challenge lies in increasing its energy density and decreasing the production cost. Higher energy density has been achieved by using electrode materials of high specific capacitance and electrolyte of larger operating voltage window. A notable improvement in performance has been achieved through recent advances in understanding charge storage mechanisms and the development of advanced nanostructured materials.

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IT-02

Magnetic Bistability in Valence Tautomers: Toward Molecular Switches

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ABSTRACT

Transition metal complexes demonstrate very interesting properties such as spin crossover (SCO), valence tautomerism (VT), mixed-valence complex and metal to ligand charge transfer. Among them, VT involves a reversible intramolecular electron transfer between the redox ligand and metal ion along with a change in the spin state of the central metal ion using an external stimulus such as temperature, pressure and light. The associated magnetic bistability in VT materials has potential applications in molecular electronic devices as molecular switches, sensors and memory storage devices.[1] In recent times, light induced excited state spin trapping (LIESST) has gained a considerable interest due to its ability to probe photo-induced metastable high spin excitation states. Even though considerable advances have been made in this field, a rational design of complexes with better photo-induced VT transition, higher conversion ratio and broader hysteresis loop remains a challenge.

In my presentation, I will discuss the role of lattice solvent and ligands in modifying the ligand field strength in cobalt bis(dioxolene) complexes. Further, our recent efforts on pressure and light induced magnetic bistability will be discussed.

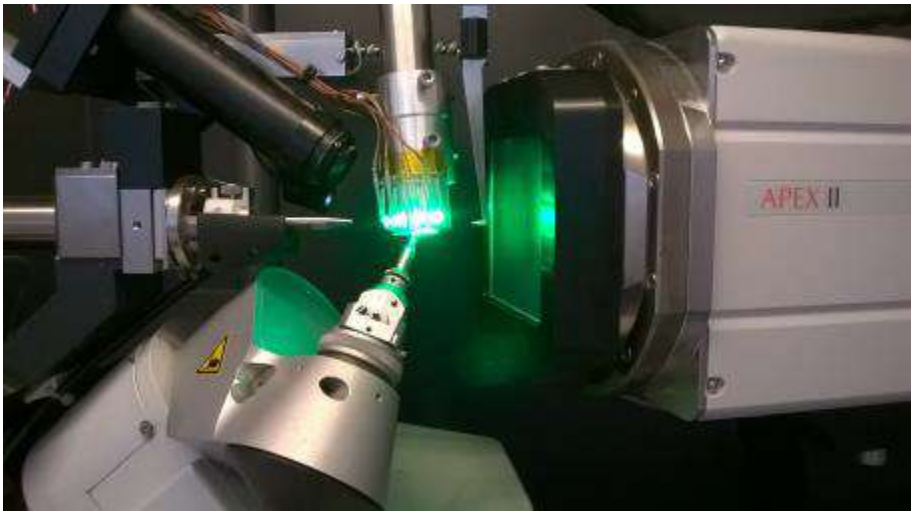

Fig. 1 : Experimental setup for photo excitation

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Generalization of Flat band Engineering in Low – dimensional Networks

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ABSTRACT

Geometrically frustrated networks supporting flat bands in their energy spectrum with macroscopically degenerate eigenstates resulting from the interplay of quantum interference and lattice topology have drawn great interest recently. The non-dispersive nature of the energy-wave vector curve causes the effective mass tensor to be divergent, leading to practically its immobility in the lattice. Such states are strictly localized either on special sets of vertices, or in a finite cluster of atomic sites spanning finite areas. Such clusters are decoupled from the rest by vertices where the amplitude of the wave function is zero. Properly modulated flat band states have divergent density of states due to the quenched kinetic energy of the particle. Such singularities in the spectral landscape are expected to produce anomalous behavior in the physical properties as well as in optical response. We demonstrate an analytically exact scheme of unraveling a multitude of flat bands in some low-dimensional structures using real space renormalization group method. Interesting competition between long range translational order in the horizontal direction and an aperiodic transverse growth leads to exotic band structures in the tight-binding formalism. These low-dispersion modes are localized over clusters of increasing size displaying the existence of multitude of localization area. The onset of localization can be delayed in space by choice of the energy of the particle. We have also described the role of uniform perturbation on flat band states.

Anderson localization is ubiquitous in diverse topic of condensed matter physics including the wave physics. Inspired by direct experimental observation of light-localization we have extended our idea of construction of such low-dispersion modes in analogy with the

electronic problem in case of fractal embedded kagome kind of wave guide network unfolding the path-breaking concept of slow light engineering which opens up the possibility of a "spatial compression of light energy" and the related nonlinear optical effects. The existence of resonant modes in the closed vicinity of such localized modes can give an interesting scenario regarding the spectral crossover. This optical analogue may inspire the experimentalists to design such network to observe the multifractal distribution of flat bands in this era of advanced nanotechnology and lithography techniques in spirit of its optical applications.

P-02

Synthesis, Characterisation and Electrical Properties of Poly (n-butyl methacrylate)/copper Sulphide Nanocomposites

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ABSTRACT

Organic-inorganic nanocomposites with an organized structure provide a new functional hybrid between organic and inorganic materials. Incorporation of nano scale constituents and organic polymeric material has been extensively studied because they continue the advantages inorganic materials (flame retardancy, modulus and thermal stability) and organic polymer (tensile strength, flexibility, ductility, modulus and processability) which are difficult to obtain from individual components. Poly (n-butyl methacrylate) (PBMA) with different concentration of copper sulphide (CuS) nanoparticles were synthesised by in situ free radical polymerization method. The formation of nanocomposite was characterised by FTIR, UV, XRD, DSC, TGA, impedance analyser and flame retardancy measurements. The shift in FTIR and UV peaks showed the intermolecular interaction between the nanoparticles and the polymer chain. The XRD studies indicated that the amorphous region of PBMA decreased with the addition of CuS nanoparticles. The SEM revealed the uniform dispersion of nanoparticle in the polymer composite. The DSC and TGA studies showed that the glass transition temperature and thermal stability of the nanocomposites were increased with the increase in concentration of nanoparticles, is due to the intermolecular interaction between the nanoparticles and the polymer. Composite with 10 wt. % of sample shows the maximum conductivity and dielectric properties than the pure PBMA is due to the increase in the ordered arrangement of nanoparticles within the PBMA chain. As the concentration of nanoparticles increased above 10 wt. %, the electrical property of the nanocomposite was decreased owing to the agglomeration of nanoparticles in the polymer. Nanoparticles could

impart better flame retardancy to PBMA/CuS composite and the flame resistance of the materials increased with the addition of nanoparticles in the polymer matrix.

P-03

Computation of DPA Cross Sections from Evaluated Nuclear Data Libraries

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ABSTRACT

The life of structural materials in a nuclear reactor is limited because of the effects due to radiation damage. It is generally quantified with a parameter called 'dpa' (displacements per atom). The dpa cross sections of neutrons are needed to compute the damage rate. For this, it is essential to know the various interactions with the lattice atoms of the target and the associated kinematics. Neutrons transfer significant amount of its kinetic energy to the lattice atoms and produces primary knock-on atoms (PKA). These recoils, during their slowing down, produce many interstitials and vacancies. The properties of materials get degraded due to these lattice defects. At IGCAR, SPECTER code based dpa cross sections are used to assess the life of fast reactors core components. It has an in-built PKA spectrum from ENDF/B-V library based on NRT model (Norgett, Robinson and Torrens). Lindhard model of energy partition between electronic and nuclear stopping is used to compute total damage energy for the secondary displacements. The present work highlights the computation methodology of dpa cross sections from the latest evaluated nuclear data libraries like ENDF/B-VII.1. The required partial cross sections and the scattering anisotropic data from the above library are used. The calculation of dpa cross sections of Fe from ENDF/B-V (Fig. 1) and its group-wise comparison with SPECTER is given in Fig.2. Results show that Fe total dpa cross section is almost equal to the sum of dpa cross sections from elastic and in-elastic reactions. The treatment of anisotropy is very important for accurate prediction of dpa cross section in higher energy.

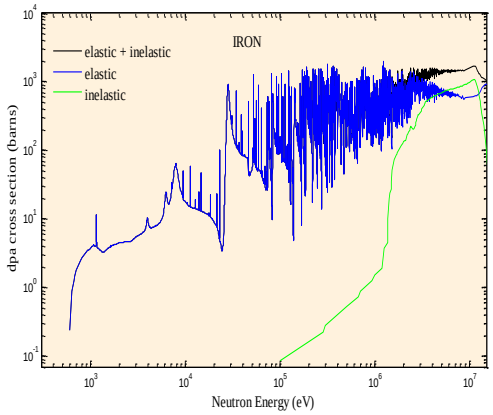

Fig. 1: *Fe dpa cross sections due to elastic and inelastic scattering reactions from ENDF/B-V*

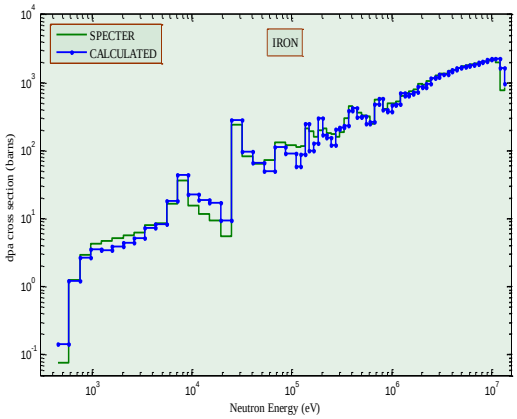

Fig. 2: *Comparison of 100-group dpa cross sections with SPECTER code*

P-04

Design and synthesis of hydrogen bonded liquid crystal from 4-undecyloxy benzoic acid and cholesteryl acetate

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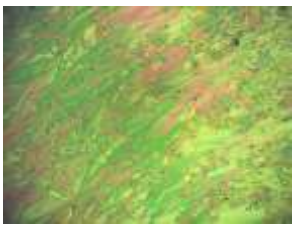
ABSTRACT

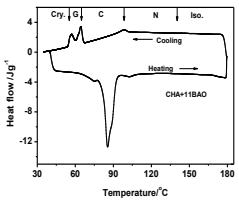
An intermolecular hydrogen bond is formed between 4-undecyloxy benzoic acid (11BAO) and cholesteryl acetate (CHA) which has been confirmed by Fourier Transform Infrared (FTIR) spectroscopic studies. Phase transition temperatures and enthalpy values are experimentally evaluated by Polarizing Optical Microscopic (POM) and Differential Scanning Calorimetric (DSC) studies respectively. An interesting feature in this paper is that the observation of wider thermal span of the mesogenic phases and decreased enthalpy values of all phases in the binary mixture compared to the individual mesogen. The resultant hydrogen bonded liquid crystal complex possesses a nematic phase with a high clearing point, and a low melting point compared to constituent in the mixture.

Nematic

Smectic C



Smectic G



DSC Thermogram

P-05

Positional influence of oxygen atom in ferroelectric double hydrogen bonded liquid crystals

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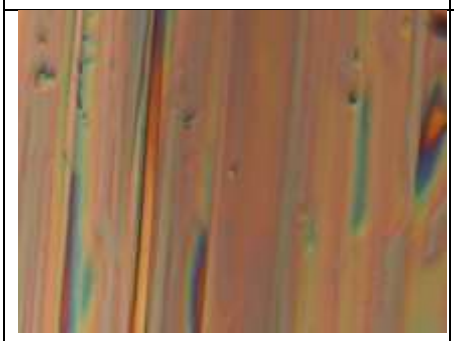
ABSTRACT

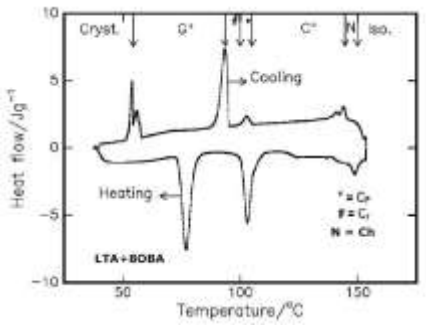
Hydrogen bond is formed between p-n-alkyloxy benzoic acid and levo tartaric acid (nOBA+LTA) while in the other it is formed between p-n-alkyl benzoic acid and levo tartaric acid (nBA+LTA). Detailed synthetic route for the same is discussed. Formation of the hydrogen bond in the complexes has been evinced through Fourier Transform Infrared (FTIR) spectroscopic studies. The positional influence of oxygen atom is investigated from the thermal and electrical characterization. It is observed that the presence of oxygen atom enhances phase abundance. To understand the influence of oxygen atom, two Hydrogen Bonded Ferroelectric Liquid Crystal (HBFLC) mesogens with same carbon number namely octyloxy complex (8OBA+LTA) and octyl complex (8BA+LTA) are chosen. The induced higher order phases such as Smectic C*, Smectic C_p* Smectic C_r* and Smectic G* have been observed in 8OBA+LTA complex where as only two phases namely, Cholesteric (Ch) and Smectic G* is observed in 8BA+LTA.

Smectic C_p^*

Smectic C_r^*



Smectic G^*



DSC Thermogram

P-06

Screening for polyphenolics rich medicinal plants using high pressure thin layer chromatographic technique

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ABSTRACT

Synthetic antioxidants such as butylated hydroxyanisole and butylated hydroxytoluene are found to be toxic, hence non-carcinogenic naturally occurring radical scavengers especially flavonoids have gained considerable importance in the past two decades. In the present study, medicinal plants from the foot hills of Western ghats are screened for its pharmacological value by considering following criteria during identification and collection: evidence for pharmacological usage of plant material by the native population, the availability of the plant in its natural habitat and sustainable use of the part(s) of the plant (root, leaves, stem, bark or whole plant). From the collected specimen, based on the literature evidence, three of the species (Rhynchosia capitata, Crotalaria globosa and Delonix elata,) are examined for its phytochemical profile. Simultaneous extraction with 95% aqueous ethanol (aq EtOH) and fractionation using solvents of increasing polarity such as benzene (C_6H_6), ethyl acetate (EtOAc) and ethanol (EtOH) of the powdered leaves and roots of R. capitata, C. globosa leaves and flowers of D. elata are carried out. The phytochemical profiles of solvent extracts of varying polarities are determined using High Pressure Thin Layer Chromatography (HPTLC). It is observed that R. capitata leaves possess highest total flavonoid content and the number of individual flavonoids present is also high. Thus HPTLC is found to be an effective tool to identify the polyphenolic composition in plants and thus can be used in screening for medicinal plants exhibiting pharmacological activity.

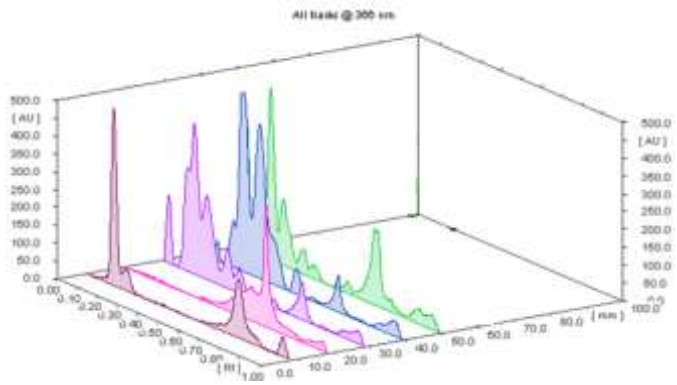

Figure 3 : D display of chromatogram of standards and samples of R. capitata leaves

P-07

Theoretical studies of hydrogen bonded alkoxy benzoic acid with suberic acid mesogen

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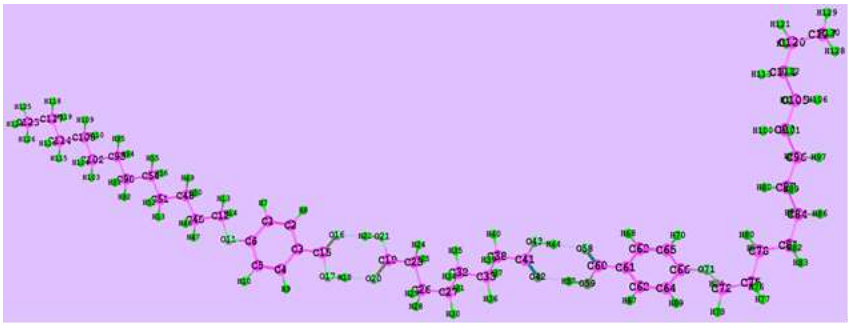
ABSTRACT

Density functional theory (DFT) is implemented for analyzing the structural properties of the synthesized 4-(dodecyloxy)benzoic acid(12OBA) with suberic acid(SA) mesogen (12OBASA). B3LYP/6-311G (d,p) basis set is adopted for all the computations carried out in the present study. The optimized geometric bond lengths and bond angles obtained by computation confirms the intermolecular hydrogen bond formation. To acquire the chemical reactivity of the molecule, the Molecular Electrostatic Potential (MEP) surface map is plotted over the optimized geometry of the molecules. MEP results shows that the negative potential sites are on electronegative atoms as well as the positive potential sites are around the hydrogen atoms. These sites give information about the region from where the reactants can have intermolecular interactions. Global and local reactivity descriptor analysis gives detailed information such as ionization potential, electron affinity, electron negativity, softness, hardness and electrophilic index reactions of the synthesized mesogens in comparison to that of individual compounds.



P-08

Effect of γ-irradiation on thermal decomposition of potassium titanium oxalate

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ABSTRACT

The thermal decomposition of pure and γ-irradiated potassium titanium oxalate (PTO) has been studied using non-isothermal thermogravimetry in nitrogen atmosphere at different heating rates. The thermal decomposition of both pure and γ-irradiated PTO undergoes through five stages forming potassium titanate. The theoretical and experimental mass loss data are in good agreement for all stages of the thermal decomposition of both pure and γ-irradiated PTO. The third thermal decomposition stage (the combined elimination of carbon monoxide and carbon dioxide) of both pure and γ-irradiated PTO were subjected to kinetic analyses by model free approach, which is based on the isoconversional principle. The results show a decrease in the value of activation energy for the third thermal decomposition stage of γ-irradiated PTO. Gamma-irradiation has little effect on all other stages of decomposition.

P-09

Photocatalytic activity and adsorption efficiency of ZnS photocatalysts

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ABSTRACT

Nanoparticles of pure ZnS have been synthesized via chemical bath deposition. The samples were characterized by X-ray diffraction (XRD), Infrared Spectroscopy (IR) and UV-Visible Spectroscopy. It is found that the formed particles are pure and nano in nature. The absorption edge in UV-Visible spectra shows that the ZnS nanoparticles undergo blue shift. The adsorption property of ZnS was studied by using Congo Red. It was found that 96% of decolorization of dye occurs within 10 minute. The photocatalytic activity of ZnS was evaluated by photocatalytic decolorization of methylene blue in aqueous solution as a model pollutant under simulated solar irradiation.

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P-10

Optoelectronic Study of Viologen Based Electrochromic Device

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ABSTRACT

In a world with ever increasing energy needs, harvesting renewable energy and using it efficiently are two of the most important energy solution strategies. One typical example is using smart windows on buildings by replacing highly glazed glass. Such installation may reduce energy consumption dramatically by reducing the cooling or heating loads, as well as the demand for electric lighting. This paper examines the properties and applications of electrochromic devices (ECD). Electrochromic materials show a change in colour on application of bias across them; hence they are of considerable technological and commercial interest because of their controllable transmission, absorption and/or reflectance. A major application of these devices is in the smart windows that can regulate the solar gains of the buildings. Other applications include anti-glare mirrors, solar cells, and small and large area display devices.

Our work is aimed at fabricating organic ECD and to investigate its properties and performance parameters. Viologen has been chosen for this purpose, due to its electrochemically reversible behaviour and the marked colour change between the two oxidation states. Our viologen based ECD exhibited adjustable transparency, low energy consumption and good repeatability. By using various electrochemical characterization techniques, I aim to investigate the optical and electronic properties of electrochromic materials and work towards the development of a device that can be commercialized in the near future.

P-11

Optical, Structural and Thermal properties of NH_4Cl/PVA polymer composites

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ABSTRACT

In recent years the proton-conducting polymer electrolytes have attracted the science and technologists due to their huge practical applications in electrochemical devices like power sources, sensors, electrochromic displays and fuel cells etc. In these materials obtaining polymer/metal complexes by the addition of metal salts to polymeric material is preferred to enhance the properties and application. It is known that the change in properties of the polymer due to doping is mainly depends on the nature of the polymer, chemical nature of the dopant and the way the dopant interacts with the polymer. In view of this in the present study a proton donar dopant NH_4Cl is doped with semi crystalline polymer PVA and the effects of doping on the PVA structure has been studied. Pure films NH_4Cl doped PVA films have been prepared by solution casting method. Optical, structural and thermal properties of pure PVA and NH_4Cl doped PVA composite films were studied using Fourier transform infrared (FTIR) spectroscopy, UV-visible, X-ray diffraction (XRD) and Thermogravimetric analysis (TGA) techniques. The observed shift in the band vibrations of the FTIR result indicates the formation of charge transfer complex (CTC). These CTC formations are due to the interaction of NH^{4+} ions with the O-H group of PVA through the inter/intra molecular hydrogen bonding. UV-Vis results show that the absorption bands of PVA shifts along with an increase in intensity. Using these results the optical energy band gaps have been estimated for various dopant concentrations and it is observed that the optical energy band gap decreases with the increase of NH_4Cl concentration. This is mainly due to the fact that the

formed CTC modified the band structure and reduce the optical energy band gap of the composite. XRD results confirmed increase in the degree of crystallinity of the composite with increase of dopant concentration and at higher dopant concentration phase separation occurred into polymer rich phase and dopant rich phase. TGA result shows the change in the weight losses of PVA composite compared to pure polymer. This study shows that the dopant modify structural, optical and thermal properties of the PVA.

P-12

Effect of deposition rate on the chalcogenide thin films prepared by chemical bath technique

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ABSTRACT

We deposited chalcogenide thin films, Copper Sulphide (CuS), Zinc Sulphide (ZnS) on different substrates by Chemical Bath Deposition Technique. Structural, Surface Morphology and Optical properties of as deposited films were investigated by XRD, SEM, FTIR and UV-VIS Spectrophotometer. The band gap is also calculated from the equation relating absorption co-efficient to wavelength. The band gap indicates the film is transmitting within the visible range and the band gaps changes because of the grain size of the films. We also observed that, the change in preparative parameters affects the deposition rate of thin films. From the observation, it is clear that the growth rate increases as the deposition temperature, deposition time, molarities of the solution increases. It is also clear that the growth rate increases as the film thickness and grain sizes increases while band gap decreases.

P-13

Effect of oxygen flow rate on sputtered NiO thin films

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ABSTRACT

We have studied the dependence of oxygen flow rate on nickel oxide thin films deposited by dc reactive magnetron sputtering at room temperature on glass substrates. The films were deposited by using a pure nickel metallic target was sputtered in the mixed ambience of oxygen and argon. Structural, electrical, optical and morphological properties of the films were investigated. X-ray diffraction reveals that films were polycrystalline in nature. Carrier type was confirmed by hot point probe method. Vander Pauw method and Hall Effect measurements have shown the films were p-type conductive with increasing carrier concentration from $2x10^{14}$ to $1.6x10^{15}/cm^3$, as oxygen flow rate increases. Mobility and resistivity of the films has decreased with increase in oxygen flow rates. Optical band gap of the films shows blue shift from 3.62eV to 3.31eV as oxygen flow rate increases. The films were semi-transparent in visible region. Surface morphology was studied by Atomic Force microscope.

P-14

Quantum chemical studies of Caffeinium bisulfate: a new non centrosymmetric form

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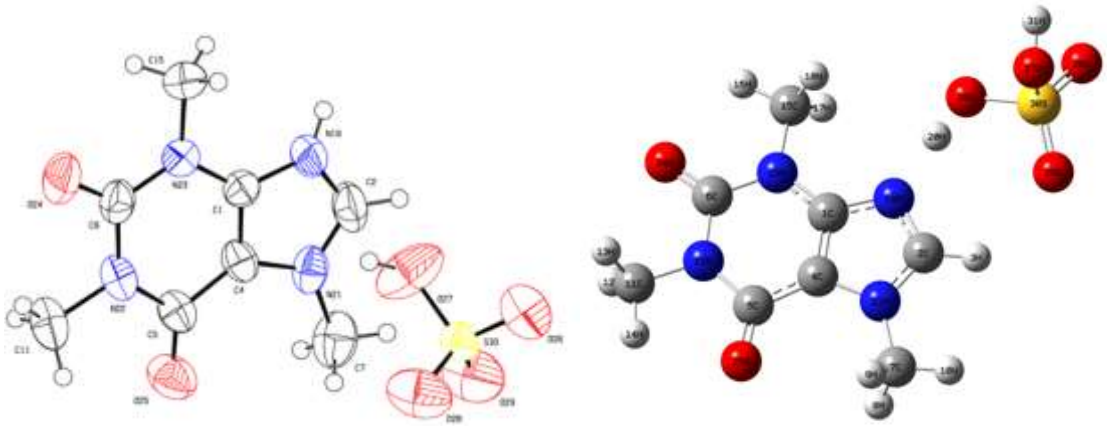
ABSTRACT

Caffeine is an alkaloid and structurally identified as 1, 3, 7-trimethylxanthine. It is one of the several xanthine derivatives which occur naturally in coffee beans, tea leaves, kola nuts and cocoa beans. It is the most widely consumed stimulant drug in the world. Caffeine is a central nervous system stimulant, a smooth muscle relaxant and commonly employed as a formulation additive to analgesic remedies. Caffeine is also a model pharmaceutical compound which exhibits instability with respect to humidity, with the formation of a crystalline non-stoichiometric hydrate.



The optimized geometries of CAFSUL molecule were obtained by both DFT and HF calculations with 6-311++G(d,p) basis set. The optimized molecular structures of CAFSUL

molecule are shown in above figure. The optimized bond lengths of C–C in pyrimidine ring fall in the range 1.376 to 1.434 Å and 1.349 to 1.439 Å in B3LYP and HF levels, respectively, with the 6-311++G(d,p) basis set. This results are in good agreement with the experimental values. The optimized C–N bond distance of caffeinium cation vary from 1.337 to 1.470 Å and 1.303 to 1.469 Å in B3LYP and HF methods respectively. The result of HF method is in close agreement with the experimental values.

P-15

Deposition of TiO_2 microflowers by aerosol assisted MOCVD

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ABSTRACT

TiO_2 has received much attention as an n-type semiconductor for optoelectronic devices, in particular dye sensitized and hybrid solar cells, and more recently for hybrid perovskite-based solar cells. For these applications, TiO_2 structures offering a high mesoporosity and surface area are especially interesting as it increases the amount of absorbed dye and concequently amount of absorbed solar energy. Using aerosol assisted metalorganic CVD (AA-MOCVD), we have developed the deposition of TiO_2 films, which contain a new kind of microstructure of TiO_2, the microflowers, around 2-3 microns of diameter. The TiO_2 microflowers are made of petals that are only several nanometers thick and oriented in different directions while the density of microflowers and of petals in each flower can be controlled by adjusting the deposition parameters. These petals are well connected to each other that could thus enhance the charge transfer through the TiO_2 network. So they should be very much effective as photoanode in Dye Sensitized Solar cell. Also this peculiar morphology could as well increase the scattering of light yielding thinner cells with better performance. Our films show another important aspect too. We have deposited the microflowers and a thin blocking later of TiO_2 beneath it in a single deposition process which can reduce both production cost and effort for making a Dye Sensitized Solar Cell. In this communication we will describe the synthesis of the microflowers and present the detailed study of their formation mechanism, properties and different characterizations. The potential integration of microflower-based TiO_2 films in functional devices will be evaluated.

P-16

Characterizations of Silicon Nanowires and Decorated Silicon Nanowires

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ABSTRACT

Nanomaterials and Nanotechnology are growing field and demand of current society and recent industry. Functional nanomaterials play fundamental roles in the development of nanotechnology, serving as novel and powerful tools for both basic studies and practical applications. Silicon nanomaterials are an important type of nanomaterials, exhibiting unique optical, electronic, or/and mechanical properties. Silicon Nanowires (SiNWs) are well known and the most important one-dimensional Silicon Nanostructures. The indirect band gap of Si (~1.12 eV), however, leads to poor optical absorption in the NIR region (750 nm < λ < 1100 nm), which hinders the development of Si photodetectors for optoelectronic and various optical based applications. Semiconducting SiNWs might enable us to overcome the limitations of conventional bulk and thin film devices because of their unique geometrical advantages. As a vertical platform of an NW array, spectral dependence of the optical response can be further modified via controlling its period, filling ratio, and symmetric arrangement.

Silicon Nanomaterials i.e here SiNWs show properties that are different from bulk materials due to their high surface to volume ratio and quantum confinement effect. Quantum confinement effect allows tranformation of energy bands into descrete energy levels due to reduced size and conversion of indirect band gap into direct band gap of silicon. This conversion of band gap gives photoluminence in visible region which gives its optical applications. SiNWs are known to possess a vastly larger optical cross-section than geometrical cross-section, due to the guided mode as well as anti-reflection effects. This leads to silicon nanowires's absorption in IR and Visible range as compared to bulk silicon

due to enhanced surface area and charge collection efficiency. If the fabricated SiNWs are decorated with metal nanoparticles i.e with noble metals, the further enhancement in absorption spectra is observed. This effect is observed due to matching of plasmon frequency of metal nanoparticles with absorption spectra of silicon nanowires. Generally the plasmon frequency of metal nanoparticles lies in visible range. This broad absorption spectrum of decorated SiNWs in IR and Visible region gives applications in solar cell applications to trap more and more light for energy conversion.

P-17

Role of NICS and shell closing model in the stability of neutral and cationic $Nb@Ge_n$ (n = 7-18) clusters: A density functional investigation

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ABSTRACT

Present investigation reports the study of the stability and electronic structures of neutral and cationic $Nb@Ge_n$ nanocluster under first principle density functional theory. From the behavior of thermodynamic and chemical parameters during the growth of these clusters it was found that neutral $NbGe_{12}$ and cationic $NbGe_{16}$ are the most stable species in the whole series of study. The $4d^4$ electrons of the doped transition metal atom Nb ($4d^4$, $5s^1$) stabilizes the majority-spin manifold, while s and p electrons of the germanium atoms enhanced the stability of the cluster via sp^3 hybridization in $Nb@Ge_n$ clusters. The enhanced stability of neutral $NbGe_{12}$ and cationic $NbGe_{16}^+$ could be explain by the negative NICS current and shell closing superatomic model with a sequence $1S^21P^61D^{10}1F^61G^42D^22S^22P^61F^81G^{14}2D^8$ respectively. These results completely matched with recent experimental paper [1].

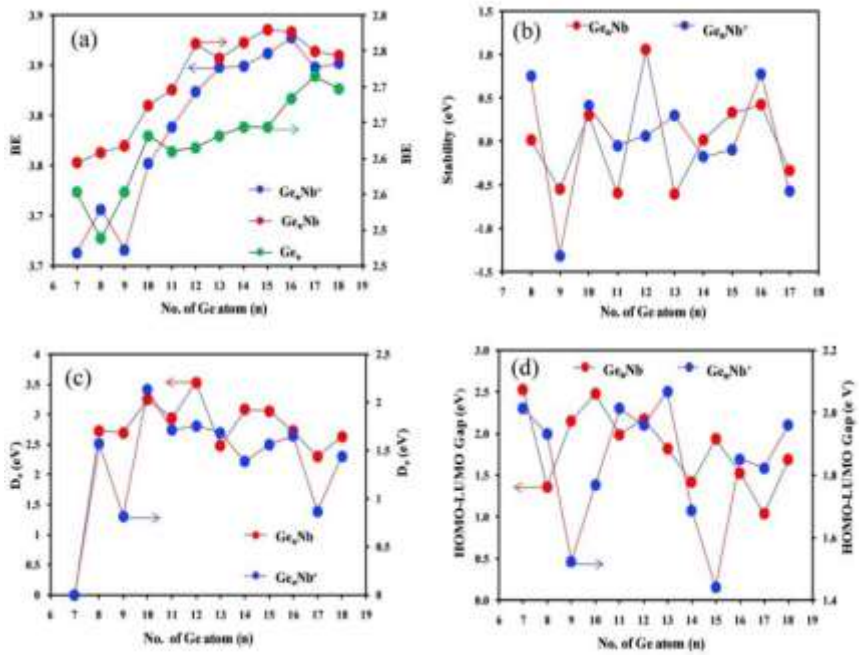

Figure 1. Variation of (a) Binding energy, (b) stability, (c) Dissociation energy and (d) HOMO-LUMO gap of $Nb@Ge_n^+$ and $Nb@Ge_n$ with the number of germanium atom.

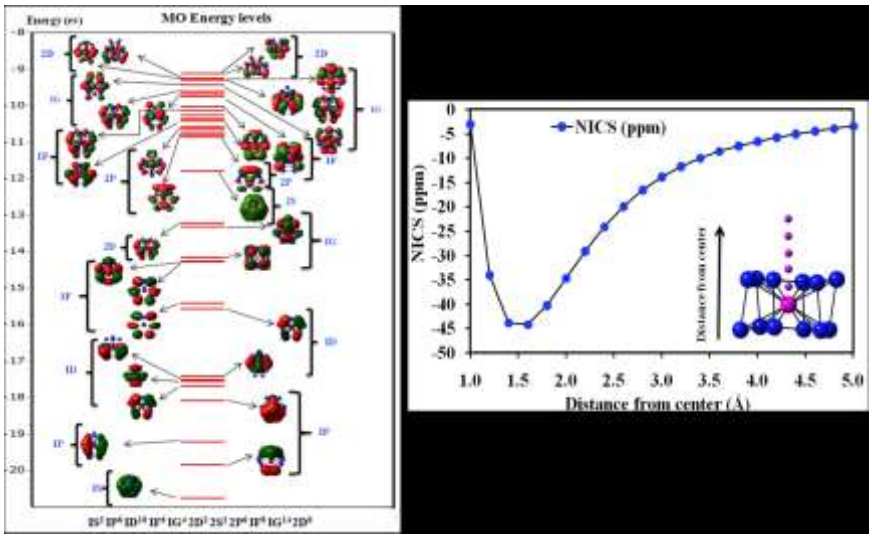

Figure 2. Superatomic orbital of $NbGe_{16}$ cationic cluster and NICS result for stable neutral $NbGe_{12}$ cluster.

Reference :

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P-18

Optically tuned light emitting polymer for plastic electronic devices

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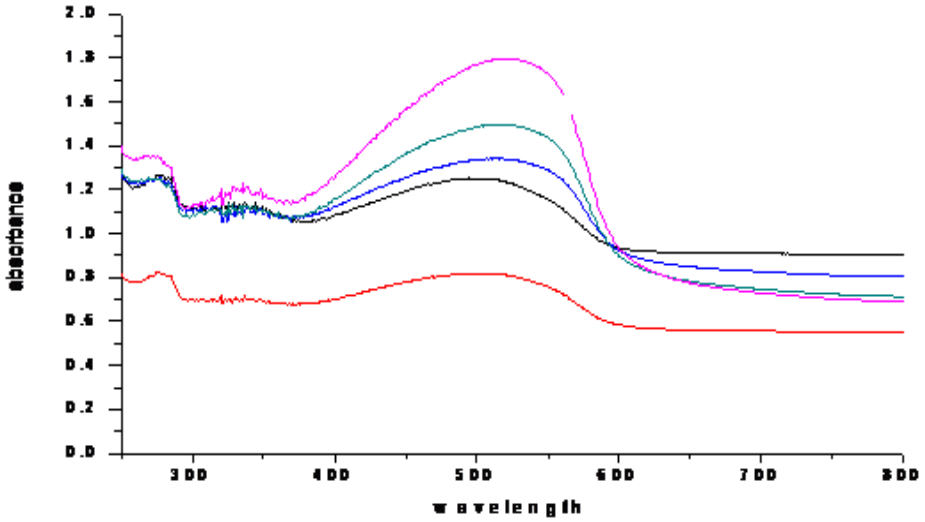
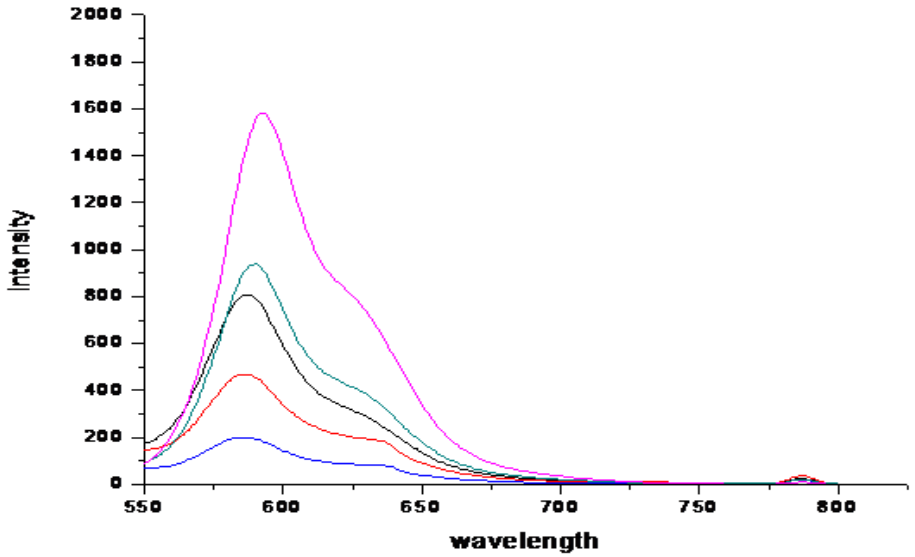
ABSTRACT

Poly [2-methoxy-5(3',7'-dimethyloctyloxy)-1,4-phenylenevinylene] (MDMO-PPV), is a light emitting polymer widely used in plastic electronic devices like LED & Solar cell. MDMO-PPV film cast from chloroform has absorption maximum at 491 nm with onset wavelength 577 nm corresponding to a band gap of 2.15 eV. The present work is focused on lowering/tuning this band gap by doping MDMO-PPV on Poly Methyl Methacrylate/Poly Vinyl Acetate (PMMA/PVAc) as the host non conducting polymer matrix. Non conducting polymer matrix is the 1:1 blend of PMMA and PVAc where in high optical transparency of PMMA and high flexibility of PVAc are incorporated in the hybrid blend. Solutions of MDMO-PPV and PMMA/PVAc are prepared in chloroform as the common solvent and films are obtained from solution cast method with MDMO-PPV doped at 0.5%, 1%, 1.5%, 2%, 2.5%, 3.0 % by weight of PMMA/PVAc film. Films are characterized by UV-VISIBLE spectroscopy, which revealed the red shift in absorption maximum. The absorption maximum (λmax) of Pure MDMO-PPV gets red shifted for MDMO-PPV doped PMMA/PVAc films, and the red shift is maximum for 3% doped film. Similar result is observed in emission spectrum (fluorescence spectrum) also. Band gap of these samples are determined which resulted in the reduction in the band gap of the MDMO-PPV. Such band gap tuned polymer films are the promising materials for electro-optics and nano-electronic devices. These new materials can be used to devise LEDs, OPVs, OFETs etc. The device construction using these new films is our further work under progress.





References:

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P-19

Structural and Optical Properties of SILAR deposited $Cd_xZn_{1-x}S$ Thin Films

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ABSTRACT

The polycrystalline chalcogenide semiconductors play an important role in photovoltaic applications. In the present research work, $Cd_xZn_{1-x}S$ thin films have been deposited on glass substrate by low cost Successive Ion Layer Adsorption and Reaction (SILAR) technique at room temperature. Aqueous solutions of cadmium chloride, zinc chloride and sodium sulphide were used as precursors for the films. The crystal structure and optical properties of the films were studied by X-ray diffractometer (XRD) and UV-Vis spectrophotometer as function of composition (x =0.1 to 0.9). The XRD patterns showed that films were polycrystalline in nature. The band-gap of the films was determined from the absorbance spectra of the films. The band gap of the films varied from 3.5 eV to 2.4 eV with respect to the composition of the films.

P- 20

Structural, optical and photocatalytic studies of CdS nanopowder

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ABSTRACT

In the past decades, the scientific and engineering interest in the application of semiconductor photocatalysis has developed exponentially. Semiconductor nanomaterials have attracted significant interest due to their tunable electronic, optical and catalytic properties arising from the quantum confinement effect. Narrow bandgap semiconductors such as CdSe, CdTe, PbS and CdS have been attracting much research attention due to their unique optical properties originating from size quantization effect. Among the various narrow band gap semiconductors, CdS with direct bandgap of 2.42 eV is suitable for light emitting devices, catalysts, optoelectronic devices and solar cells applications. In the present study, CdS nanoparticles have been synthesized by chemical precipitation method. As-synthesized nanoparticles were characterized by XRD, SEM with EDS, TEM, FT-IR, optical absorption, photoluminescence and photocatalytic activity. XRD results reveal the hexagonal phase of CdS and the average crystallite size is evaluated using Scherer's approximation as 23 nm. SEM and TEM micrographs shows spherical like structures. EDS spectrum shows only the target elements, Cd and S species. FT-IR spectrum confirms the formation of CdS with stretching vibrational mode at 621 cm^{-1}. Photoluminescence spectrum shows broad emission in green region. Photocatalytic efficiency of the prepared CdS nanopowder on the photodegradation of azo dyes (methylene blue and rhodamine-B) have been studied and a plausible mechanism for the synergetic photocatalysis has been discussed in detail.

P- 21

Pressure Dependent Structural, Electronic, Vibrational Spectroscopy of Platinum Oxide Using First Principle Calculation

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ABSTRACT

In present work, we reports a density functional theory study of the atomic structure of bulk PtO and study the electronic and vibrational spectroscopy of bulk PtO has determine by the perdew-Burke-Ernzerhof (PBE) exchange-correlation functional at compressive pressure in the interval of 10 GPa and thermodynamic properties of the bulk tetragonal PtO structure. The calculated electronic band structure of PtO show that poor metallic behaviour with very low densities of states at the Fermi level. Here, we can see that the stability of structure through phonon dispersion curve and Raman peaks both slightly shifted higher frequency as applying pressure, but the intensities of the Raman peaks has been decrease as applying pressure. As mention below, there is six Raman active modes are present in Raman spectra. Our work characterized observed all the peaks of Raman active modes and stability of the bulk tetragonal PtO structure. We have calculated the pressure dependence study of thermodynamics properties such as entropy, specific heat at constant volume, enthalpy and Gibbs free energy. It is used as sensors, photo-cathode in water electrolysis, for thermal decomposition of inorganic salt and fuel cells. which are expected to play an important role in catalysis.

P- 22

Preparation and Characterization of New Thermoelectric Materials

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ABSTRACT

The polycrystalline samples of $Mn_{50-x}CoGa_{25+x}$ and $Ga_{50-x}MnCo_{25+x}$ have been prepared using Tri-Arc melting technique. The phase purity of the prepared samples is confirmed by powder x-ray diffraction experiments followed by Rietveld analysis. Transport properties of the samples have been studied at low temperature resistivity measurement setup using four-probe method. It is observed that there is metallic behavior in all samples and it is found that there is a magnetic phase transition in some samples, a non-magnetic behavior in other sample and the transition shifts from higher to lower temperature with different x. Our result will specify how the band structure at Fermi level is related to thermoelectric properties of the samples which may help in designing Mn, Co based thermoelectric material and spintronic devices.

P- 23

Molecular dynamical study of thermal conductivity of nanoparticles

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ABSTRACT

A model has been used to estimate the theoretical thermal conductivity of fcc metal nanoparticles by Molecular dynamical simulations. The Molecular dynamics (MD) simulation of heat transfer through nanoparticles of different dimensions and initial temperatures in contact with giant heat source shows different temperature evolution at different position. The extent of temperature rise was found to depend on the distance as well as the time of heat transfer by conduction mode. It is observed that the reduction of particle size down to nanometre range reduces the thermal conductivity to a great extent. The high specific surface area of nanoparticle reduces the effectiveness of phonon transfer as compared to bulk material particles. It is observed that nano dimensional thermal conductivity of Cu is of the same order for Al and Ag nanoparticles. The reduction of phonon wave due to reduction of particle size may be responsible for this effect. The estimated value of the thermal conductivity of nanoparticle has been compared with the literature available, in order to get an idea about the effect of reduction of size of particles down to nanometre range on the thermal conductivity.

P- 24

Influence of Rapid Thermal Annealing on Electrical Characteristics of Au/Y/p-InP/Pt Schottky Barrier Diode

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ABSTRACT

The rapid thermal annealing effects on the electrical properties of Au/Y/p-InP/Pt Schottky barrier diode (SBD) have been investigated using current-voltage (I-V) and capacitance-voltage (C-V) characteristics. The measured barrier height (BH), ideality factor (n) of as-deposited and 200 oC annealed Yb/p-InP/Pt SBD are found to be 0.62 eV (I-V)/0.83 eV (C-V), 1.32 and 0.63 eV (I-V)/0.92 eV(C-V), 1.23 respectively. Results showed that the BH increases to 0.65 eV (I-V)/0.96 eV (C-V) and ideality factor decreases to 1.19 upon annealing at 300 ^{o}C for 1 min in N_2 atmosphere. However, the BH slightly decreases to 0.59 eV (I-V)/0.78 eV (C-V) and ideality factor (n) increases to 1.48 after annealing at 400 ^{o}C. Also, the discrepancy between the barrier height obtained from C-V and I-V characteristics is discussed. The modified Norde method is also used to evaluate the BH and series resistance (RS) of Au/Y/p-InP/Pt SBD and the corresponding values are 0.71 eV and 125 Ω for as-deposited, 0.75 eV and 59 Ω for 200°C, 0.78 eV and 67 Ω for 300°C, and 0.64 eV and 69 Ω for 400°C respectively. Furthermore, Cheung's functions are used to extract the BH and series resistance (R_s) of the Au/Y/p-InP/Pt SBD at different annealing temperatures. The series resistance (R_s) is calculated by Cheung's functions and the corresponding values are 50 Ω and 64 Ω for as-deposited, 33 Ω and 42 Ω for 200 °C, 30 Ω and 36 Ω for 300 °C, and 37 Ω and 51 Ω for 400 °C from the dV/d(lnI) versus I and H(I) versus I plots, respectively. In addition, the energy distribution of interface state density (N_{ss}) is determined from the forward bias I-V characteristics by taking into account the bias dependence of the effective BH. The interface state density is calculated for the as-deposited Au/Y/p-InP/Pt SBD is 2.0671×10^{12} $eV^{-1}cm^{-2}$, 1.5543×10^{12} $eV^{-1}cm^{-2}$ for 200 ^{o}C, 1.1955×10^{12} $eV^{-1}cm^{-2}$ for 300 ^{o}C and

2.5310×10^{12} $eV^{-1}cm^{-2}$ for 400 ^{o}C respectively. Based on the above results, the interface state density (N_{ss}) and series resistance (R_s) play a significant role on the electrical characteristics of Au/Y/p-InP/Pt Schottky barrier diode.

P- 25

Photoluminescence properties of praseodymium doped fluoro-phosphate glasses for solid state lighting applications

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ABSTRACT

Five fluoro-phosphate glasses of different compositions, $49.5P_2O_5$ -$10AlF_3$-$10BaF_2$-$10SrF_2$-10PbO-10M (M= Li_2O, Na_2O, K_2O, ZnO and Bi_2O_3) doped with 0.5 mol% praseodymium were prepared by melt quenching technique and studied their luminescence properties. X-ray absorption near edge spectroscopy (XANES) was used to study the electronic structure of praseodymium in the host glass matrices. By analyzing the absorption spectra with Judd-Ofelt theory, three intensity parameters (Ω_λ, λ=2, 4, 6) are obtained. In turn these parameters are used to calculate radiative properties such as emission probabilities (A_R), radiative lifetimes (τ_R) and integrated absorption cross sections (Σ) of different Pr^{3+} transitions. Luminescence parameters such as stimulated emission cross-sections (σ_p) and branching ratios (β_{exp}) have been studied through photoluminescence spectra. Further, decay time constants are estimated from the decay profiles of Pr^{3+} doped different fluoro-phosphate glasses.

P- 26

Synthesis and Characterization of Sodium Potassium Niobate Doped Polymer composite films

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ABSTRACT

Sodium Potassium Niobate ($Na_{0.5}K_{0.5}NbO_3$) ceramic was prepared through conventional solid state reaction route using AR grade $NaNO_3$, KNO_3 and Nb_2O_5 in stochiometric ratio. Poly vinyl alcohol (PVA) polymer - Sodium Potassium Niobate composite films was prepared by solution casting method by changing the blend ratio of PVA / $Na_{0.5}K_{0.5}NbO_3$ (100:0, 90:10, 75:25, 50:50). The prepared samples in the form of films were characterized by powder X-ray diffraction. The XRD studies revealed the presence of both ceramic and polymer phases in prepared PVA- Sodium Potassium Niobate composites. The composite films were also investigated through SEM studies and SEM surface morphology of these films revealed crystallites are distributed in polymer matrix and the porosity is almost negligible. The ac conductivity of these samples were also studied at room temperature.

P- 27

A Review on Overlay method

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ABSTRACT

We report how microstrip ring resonator (MSRR) will helpful to explore the dielectric properties of materials using overlay method (A resonant method). The interaction of electromagnetic waves with matter is governed by its complex permittivity. The dielectric constant and loss tangent of materials are important inputs to RF engineering tasks. Knowledge of the dielectric constant and loss tangent of a dielectric material is required to understand how that material will reacts with electromagnetic fields and behave in RF circuits. Dielectric permittivity measurements provide important input to engineering and scientific disciplines due to the effects of permittivity on the interactions between electromagnetic energy and materials. Every material has a unique set of electrical characteristics that are dependent on its dielectric properties. Accurate measurements of these properties can provide scientists and engineers with valuable information to properly incorporate the material into its intended application for more materials designs.

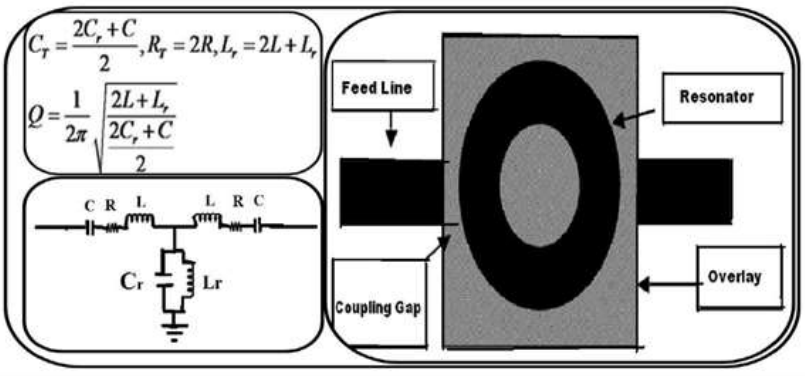

Figure 1. Schematic structure, equivalent lumped circuits of MSRR.

P- 28

Preparation and Characterization of Porous Hydroxyapatite Scaffolds Through Slip casting and Robocasting Methods

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ABSTRACT

Hydroxyapatite a synthetic calcium phosphate has been considered as a potential bioceramic material since many years due to its similarity to the inorganic constituent of bone mineral and hence good biocompatibility. Fine hydroxyapatite powder was synthesized through solution combustion reaction using glycine as fuel. The powders were characterized for crystalline phase, particle size, morphology and surface area. The powder has particle size in the range of 100-200nm and surface area of 14-16m^2/g. Porous samples of this hydroxyapatite were fabricated using slip casting and robocasting methods. The required slurry was prepared by homogeneous mixing of the powder with de-ionized water and a dispersant through the ball milling process for 16-20 hrs. The slurry was characterized by studying the viscosity and rheology. Slip casting was carried out in plaster moulds and the robocasting follows extrusion through a fine nozzle and deposition in X. Y, Z direction through a 3 dimensional dispensing machine. The cast samples were sintered at 1250°C for 1 hr and the sintered samples were characterized in terms of density, porosity, microstructure, and mechanical properties. The results show that scaffolds obtained has porous microstructure including micro and macro porosity. These porous structures are intended to be used as scaffolds in bone tissue engineering applications.

P- 29

Preparation and characterization of indium telluride thin films

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ABSTRACT

Indium telluride (In_2Te_3) thin films were synthesized using thermal evaporation method, followed by post annealing process. The structure, surface morphology and composition of the grown films were studied by X-ray diffraction, scanning electron microscope and energy dispersive analysis respectively. The obtained films were cubic in structure with lattice constant a = 18.478 Å. The films were homogeneous and nearly stoichiometric. Optical transmittance measurements revealed the existence of direct and indirect transitions. Resistivity and the temperature dependence of resistivity have been studied to evaluate the thermal activation energy for conduction in the films. Carrier concentration calculated using Hall Effect experiments indicate the carrier concentration to be of the order of 10^{20} m^{-3}.

P- 30

Structural and Optical properties of Thermally Evaporated ZnS Thin films

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ABSTRACT

In the recent years, the II-IV semiconductors have found significant importance in fabrication of opto-electronic devices. In the current work, ZnS thin films were coated on glass substrates in vacuum by resistive heating technique. The crystal structure and optical properties were studied using X-ray diffractometer (XRD) and UV-visible spectrophotometer respectively. XRD patterns showed that the films were polycrystalline in nature and exhibited cubic structure. Grain size and microstrain of the films were calculated. Optical bandgap was measured close to 3.5 eV.

P- 31

Effect of anionic and cationic dopants over structural and optoelectronic properties of wide band gap metal oxide semiconductors

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ABSTRACT

Zinc oxide and tin oxide have drawn interest in recent times for their optoelectronic properties in the replacement of ITO (Indium Tin oxide). In this paper Zinc oxide and Tin Oxide powders were synthesized using simple sol gel process. The effect of anionic and cationic dopants like Fluorine, Aluminum and Zinc over the structural, optical and morphological characteristics were investigated. The synthesized powders were dried and annealed at 300˚C. XRD spectra revealed that the synthesized powders were highly polycrystalline in nature and also found exactly matching with the standard spectra for Wurzite ZnO (ICDD no: 36-1451) and Rutile SnO_2 (ICDD No. 45-1445). Morphological studies showed that high temperature annealed samples possess uniformly distributed spherical shaped particles. UV-Vis absorbance spectra were recorded for all the powder samples. Band gap analysis (hv vs $(\alpha hv)^2$ plot) revealed increasing trend from 3.28 eV (ZnO) to 3.33eV for Fluorine doped crystalline ZnO and from 3.4eV (SnO_2) to 3.51eV for Zinc doped Tin oxide.

P- 32

Structural and dielectric properties of hydrothermally synthesised ZnS

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ABSTRACT

ZnS is one of the most important II-IV semiconductors finding applications in solar cells, optoelectronics and photonic crystals. Nanosized ZnS has been synthesised using zinc acetate dihydrate and thioacetamide (TAA) as precursors by conventional heating. Crystal structure, size and strain produced in the nanocrystallites is determined by X-ray diffraction. Frequency dependent variations of relative dielectric constant, dielectric loss and ac conductivity are studied at room temperature. The ac conductivity appears to follow frequency dependent power law: $\sigma_{ac}=A\omega^{s}$ with $0 < s < 1$. Correlated barrier hopping CBH) model explains the room temperature conduction in the sample and the barrier height is also estimated.

P- 33

Growth and Characterization of spray deposited Gallium Doped SnO_2 Thin Films

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ABSTRACT

Transparent SnO_2 films and gallium doped SnO_2 have been deposited on glass substrate using spray pyrolysis. Tin (ii) chloride dihydrate and Gallium (iii) chloride were used as a precursor for SnO_2 films and Ga doped SnO_2 films respectively. The deposition of the films as function of substrate temperature, flow-rate, spray-time, film thickness and annealing effect has been studied. X-ray diffraction (XRD), scanning electron microscope (SEM) and energy dispersive X-ray analysis (EDAX) were used for structural, surface morphological and compositional characterization. The XRD analysis revealed that the synthesized films were tetragonal in structure. Doping of SnO_2 films was observed to reduce the crystallinity of the films. The SEM studies confirm the formation of homogeneous and uniform films. Optical transmittance and electrical conductivity of the films were evaluated using UV-Visible spectroscopy and two probe method respectively. The optical studies showed that the SnO_2 thin films have high optical transmittance >80% in entire visible region. The resistivity of undoped films were approximately 10^{-2} Ωcm and doping was observed to marginally increase which is explained as due to the reduction in crystalline quality.

P- 34

Theoretical first order molecular hyperpolarizability and Experimental second harmonic generation studies on novel nonlinear optical material: L-histidinium p-toluenesulfonate [LHPT]

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ABSTRACT

L-histidine, an amino acid, is well known for its NLO behaviour for the past few decades. From the literature, the list of such L-histidine based materials are identified to be L-histidine acetate, L-histidine chloride monohydrate, L-histidine tetrafluoroborate, L-histidine hydrochloride monohydrate, L-histidine hydrofluoride dihydrate, L-histidine bromide and L-histidinium trichloroacetate. The nonlinear optical property in these materials is perceived due to the inherent molecular chirality of the amino acid molecule. The requirement of better nonlinear optical (NLO) materials with enhanced properties is increased rapidly due to the development in laser-based imaging, communication, optical data storage and counter measure systems.

The first order hyperpolarizability calculation was done by the RHF method using Gaussian 09W [29] program package with two different basis sets, viz., 6-31++G(d,p) and 6-311++G(d,p). The calculated dipole moment (μ) and the first order hyperpolarizability (β0) of the compound are 4.937 & 2.171 Debye (D) and 7.535 & 3.033 × 10^{-30} esu with different basis sets respectively. The first order hyperpolarizability of the title compound is 3.1 times

[6-31++G(d,p)] and 1.25 times [6-311++G(d,p)] greater than the KDP (μ and β0 of KDP are 3.151 Debye and 2.423 × 10^{-30} esu). The present molecular assembly has large first order hyperpolarizability due to the intramolecular charge transfer. The larger dipole moment of the compound is due to the delocalization of oxygen lone pair of electrons into the p-toluenesulfonate. The SHG efficiency of grown LHPT was measured by Kurtz and Perry powder technique. It reveals that the SHG efficiency of the present compound is 1.8 times greater than the KDP.

P- 35

Luminescence Studies on Lanthanide ion (Eu^{3+}) doped $CaLaAlO_4$ Phosphors Materials

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ABSTRACT

A trivalent rare earth ion doped Calcium Lanthanum Aluminate (CLA) phosphor of composition $CaLa_{1-x}AlO_4$: xEu_2O_3 (x = 0.01, 0.03 and 0.05 mol %), were prepared by the conventional solid state reaction method at 1100^oC. Materials were characterized by powder XRD, FTIR and SEM-EDS techniques. The luminescence properties of these Eu^{3+}:$CaLaAlO_4$ materials were also investigated. The emission spectrum of these samples shows a typical spectrum of the Eu^{3+} in between 585 to 700 nm ($^5D_0 \rightarrow {}^7F_{j=0,1,2,3}$) may be attributed to the 4f-4f intra shell transitions. The results indicated that $CaLaAlO_4$:Eu^{3+} material is a promising red phosphor for the application as near-UV/blue light-pumped w-LEDs and also point to its use in new color light sources, fluorescent display devices and optoelectronic devices.

P- 36

Polyaniline-coated graphite oxide composites for broadband electromagnetic interference shielding

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ABSTRACT

There is an ever increasing demand for high-performance electromagnetic interference (EMI) shielding materials due to the rapid proliferation of electro/electrical systems. This study presents the investigations on EMI shielding and microwave absorption properties of polyaniline-coated graphite oxide (PAni/GO) composites. The spectroscopic characterizations of the composites were performed using X-ray diffraction (XRD), scanning electron microscopy (SEM) and high resolution transmission electron microscopy (HRTEM). The EMI shielding measurements were carried out in the frequency range of 12-18 GHz (Ku-Band), relevant for practical applications. The shielding analysis demonstrates the synergistic effect of the complementing phases (i.e. PAni and GO) which leads to high shielding effectiveness (SE) in the range of –38 to –46 dB (< 99.99 % attenuation). The higher shielding effectiveness and the possibility to tailor the properties of these composites by varying the concentration of graphite oxide content can be optimized for making effective broadband microwave shields.

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Synthesis, Growth and Structural Characterization of a Novel Chalcone Compound

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ABSTRACT

A new chalcone derivative (2E)-3-(2,3-dimethoxyphenyl)-1-(3-nitrophenyl)prop-2-en-1-one (3DPNP) has been synthesized and grown as a high-quality single crystal by the slow solvent evaporation technique. The crystals were structurally characterized by FT-IR, NMR and XRD techniques. FT-IR and NMR confirms the functional groups present and purity of the sample. XRD studies reveal that the compound crystallizes in the monoclinic system in a centrosymmetric space group P 2_1/n. Thermal analysis shows that the crystals are thermally stable up to the temperature of 142˚C. The optical absorption study reveals the transparency of the crystal in the entire visible region. The potential of these crystals for non-linear optical (NLO) applications were studied using molecular hyperpolarizability calculations using MOPAC 2012. The results show that the structure of the compound has great impact on NLO properties and can be a promising candidate for optical device applications.

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Synthesis and Characterization of Graphene Oxide - Polyoxometalate Composite Material for Device Applications

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ABSTRACT

Polyoxometalates (POMs) consisting of clusters of d-block transition metals and oxygen atoms represent an important class of water soluble polynuclear nanomaterial. The tuneable size, structure and elemental composition of POM draws considerable attention for the development of functional composite materials of desired chemical and electronic properties [1]. Graphene can be the promising support for POMs due to its low band gap energy and fast electron transport properties. These properties of grapheme facilitates transport of electrons of POMs rapidly and effectively [2]. In the present investigation, graphene oxide (GO) and reduced graphene oxide (rGO) have been used as a support for POM-graphene composites for semiconductor, hydrogen production applications [2]. The deposition of POM on graphene oxide sheets were carried out through electron transfer interaction and electrostatic interaction between POM and GO sheets. The interaction between polyoxometalate and the GO sheet was confirmed using various characterization techniques such as FTIR, Raman spectroscopy, UV-vis spectroscopy, powder XRD, SEM, and TEM. Detailed characterization results confirmed deposition of POM cluster on graphene. The POM-graphene composite were explored as active materials for memory device applications.

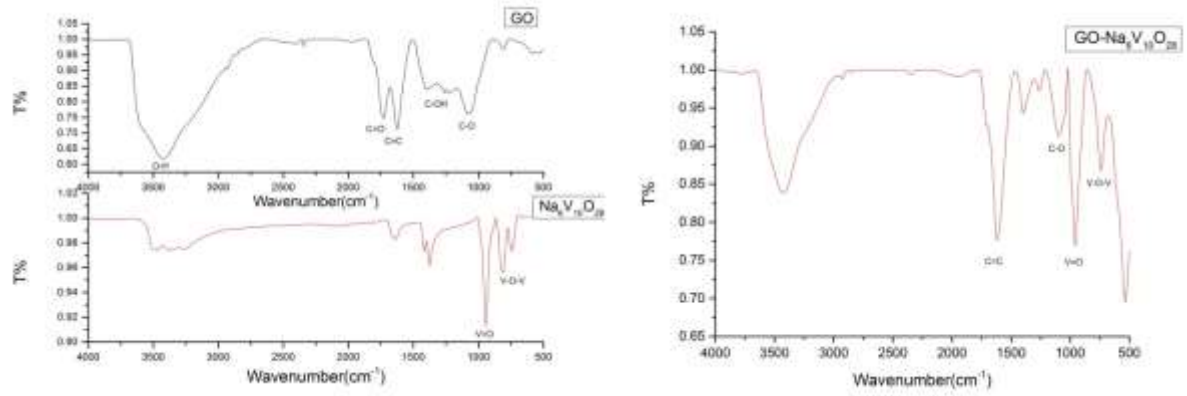

Figure: FT-IR spectrum of GO, $Na_6V_{10}O_{28}$ and GO- $Na_6V_{10}O_{28}$

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Investigation of third order optical nonlinearity of novel chalcone derivative 3-(4-fluorophenyl)-1-(3-Nitrophenyl)prop-2-en-1-one through z-scan technique

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ABSTRACT

A novel chalcone derivative 3-(4-fluorophenyl)-1-(3-Nitrophenyl)prop-2-en-1-one abbreviated as F3NC synthesized using Claisen-Schmidt condensation reaction method. Single crystals of F3NC were grown using slow evaporation technique. The optical transmittance window and the lower cutoff wavelength of the F3NC have been identified by UV-VIS studies. The third order nonlinear optical properties of grown crystals have been studied using single beam z-scan technique with continuous wave DPSS (Diode pumped solid state) laser operating at 532nm wavelength and 200mW power. The calculated values of nonlinear R.I, nonlinear absorption coefficient and magnitude of third order susceptibility are of the order $-2.44 \times 10^{-7} cm^2/W$, $2.25 \times 10^{-4} cm/W$ and 2.085×10^{-5} e.s.u respectively. The second order hyperpolarizability value obtained is of the order 8.6×10^{-25} e.s.u. The crystal shows optical limiting behavior with limiting threshold of 950.25 J/cm^2. The results suggest that this material is considered as a promising candidate for future optical devices applications.

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Effect of oxygen flow rate on dielectric and structural properties of DC reactive magnetron sputtered ZrO_2 grown thin films at room temperature

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ABSTRACT

Zirconium oxide thin films were deposited on the p-type Si substrates by DC reactive magnetron sputtering at room temperature. We investigated the structural, morphological, optical and electrical properties of ZrO_2 thin films for gate dielectric application at different oxygen flow rates. The XRD analysis reveals that the deposited films show a nanocrystalline phase. Study of surface roughness of the film was carried out using AFM method which shows an increase in the surface roughness with an increase in oxygen flow rates. For the electrical characterization we have constructed MOS capacitor with Aluminum as a metal electrode. From this we observed that leakage current density decreases and dielectric constant increases as the oxygen flow rates increases. The leakage current density of $10^{-8}A/cm^2$ and dielectric constant of 26.8 was achieved from this optimization. The flat band voltage, fixed oxide charge density and interface trap density were found out using conductance method and its variation was studied with the change in oxygen flow rates.

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Structural, morphological and optical properties of ZnO doped Tungsten oxide thin films

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ABSTRACT

Among the transition metal oxides, WO_3 is the most widely used one in thin film form because of its wide variety of technological applications such as smart windows, display devices, memory devices etc . Recently, many efforts have been devoted to the investigation of tungsten oxide nano materials. Undoped and ZnO doped WO_3 films with different ZnO doping concentrations viz. 0.5, 1, 3 and 5 wt % are prepared on quartz substrate using RF magnetron sputtering technique and the films are annealed at a temperature of 600^0C for 1hr. The structural, morphological and optical properties of the undoped and ZnO doped WO_3 films are studied using techniques like XRD, AFM, FESEM, EDS, micro-Raman and UV-Vis spectroscopy. The XRD patterns shows polycrystalline nature presenting the monoclinic phase of WO_3 (JCPDS Card No. 83-0951) in all the films. The highest intensity of the (0 0 2) peak suggests that <2 0 0> is the preferred direction of crystalline growth in all the films. A systematic increase in the XRD intensity and a systematic decrease of FWHM of the (0 0 2) peak with increase in ZnO doping concentration suggests the enhancement of crystallinity with ZnO doping. In films with ZnO doping concentrations 3 and 5 wt% an additional peak around 30.50 corresponding to monoclinic phase of $ZnWO_4$ (JCPDS Card No. 73-0554) is observed. Raman spectra also support the formation of $ZnWO_4$ in WO_3 films with high ZnO doping concentrations. The surface morphology depicted by AFM and SEM images shows a dense distribution of well-defined grains in all the films. All the films exhibit high transmittance of the order of 78-83 % in the wavelength region 400-900 nm. In the present work a band gap renormalisation in tungsten oxide with ZnO doping is observed.

Band gap energy shows a systematic decrease from 3.13 to 2.70 eV with increase in ZnO doping concentration making the films suitable for solar cell applications.

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Synthesis, Structural, Morphological and Nonlinear optical property of $BaSnO_3$

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ABSTRACT

$BaSnO_3$ is a cubic perovskite-type oxide that behaves as an n-type semiconductor with a wide band gap of 3.4 eV and remains stable at temperatures up to 1000^0C. $BaSnO_3$ powder was prepared by solid state ceramic method. The structural, morphological and optical properties of the material were investigated in detail. The XRD pattern of $BaSnO_3$ powder prepared by solid state reaction presents a polycrystalline nature. X-ray diffraction pattern of the prepared sample presents all the characteristic peaks of cubic phase of $BaSnO_3$ (JCPDS card no: 15 - 0780). The lattice constant for the compound was calculated and found to be $4.101A^0$ which is in agreement with the reported value ($4.112A^0$). Barium stannate in the cubic structure has space group Pm3m with 1 formula unit per Bravais lattice. The Raman bands observed ~ 139, 833 and 1122 cm^{-1} can be assigned on the basis of the fundamental vibrations of SnO_6 octahedron which has O_h symmetry, in the distorted perovskite structure. The Raman active mode observed at $139cm^{-1}$ can be assigned tov_5F_{2g} mode. The SEM image shows a porous surface morphology with grains of cuboidal structure having well defined grain boundaries.

The sample exhibit high reflectance in the 400-700 nm range. The band gap energy is found to be ~ 3.1eV which is in agreement with reported values. Thermo-emf is found to be negative for the sample over the entire temperature range of measurements. The Z-scan data can be used to plot the variation of sample transmission with input laser fluence. The open aperture Z-scan measurements are carried out in the present sample using 5 ns laser pulses at 532 nm from a frequency doubled Nd: YAG laser (MiniliteI, Continuum). The normalized transmission decreases at higher laser intensities indicating an optical limiting behavior. These values indicate a high optical limiting efficiency, comparable to that of graphene and its metal hybrids.

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Transport properties of Polyaniline / TiO_2 Nanocomposite

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ABSTRACT

Transport properties (V-I characteristics and Hall Effect studies) of Polyaniline, core-shell structured TiO_2/Polyaniline Nanocomposite are studied at room temperature. The V-I characteristic of conducting Polyaniline salt form follows non-ohmic relation. Here charge conduction is not only carried by free carriers (electron & hole) such as in intrinsic semiconductors but also is carried by the formation of polarons and bipolarons. Volt-Ampere measurements were also performed on the TiO_2 /PANI core-shell structured nano-composite. The V-I characteristics results imply that additional current transport mechanism dominate in the composite. Current-voltage characteristics of PANI and PANI/TiO_2 can be expressed as $I = KV^m$. The exponent m is ~1 for Emeraldine base form, 1.66 for PANI ES form and 1.76 for PANI/TiO_2. The Hall Effect studies are providing valuable information regarding nature of the charge carriers, Hall Voltage, Hall Coefficient (R_H), carrier density (n) and carrier mobility (μ) of the material. In application part Polyaniline and TiO_2 hetero-junction have been fabricated for rectification.

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SANS and DLS Studies on Core-Shell Structured Polyaniline/TiO_2 Nanocomposite

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ABSTRACT

Among the conducting polymers, Polyaniline (PANI) is a promising material with high environmental stability and electrical conductivity. It is a unique polymer which can be synthesized with tunable electrical conductivity; one of the prominent quotations given by Prof. A.G. MacDiarmid is that "There are as many different types of PANI as there are people who synthesize it". Similarly there has been a great deal of interest in making Polyaniline-based inorganic-organic Nanocomposite because the impregnation of inorganic materials into a polymer matrix can introduce new properties to polymers as well as to the inorganic materials. Here we synthesized TiO_2 and Polyaniline/TiO_2 nonocompistes by sol-gel and in-situ method Chemical polymerization of aniline with ammonium peroxide as oxidant. We established the core-shell structure morphology between TiO_2 and Polyaniline with help of XRD, SEM, TEM, Small angle neutron scattering (SANS) and Dynamic Light scattering (DLS). These results indicate that the Polyaniline shell is formed with around 19 nm shell thickness on the 55 nm TiO_2 nanoparticles.

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Fabrication of Bi-layer structured Poly L-Lactide (PLLA) – Polyvinylpyrrolidone (PVP) / TiO_2 composite for food packaging

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ABSTRACT

Research and development of biocompatible and biodegradable polymer composites for food packaging applications is a subject of great commercial interest. The need and the expectation of the society are towards the improved quality, safety and the extended shelf lives. Therefore, in the present work bi-layer ultra-thin fiber scaffolds of Poly L-Lactide (PLLA), Polyvinylpyrolidone (PVP) were prepared using chloroform and ethanol-water mixture as solvents by utilising electrospinning technique. The Anatase TiO_2 nanoparticles synthesized by sol-gel method were incorporated into the hydrophilic PVP for its effective use as an antibacterial agent. The bi-layer structure was prepared in which one layer constitutes the hydrophobic PLLA ultra-thin fibers and the successive layer contains the hydrophobic TiO_2 nanoparticles incorporated PVP ultra-thin fibers. The electrospun fibers were characterised using Scanning electron Microscopy, Infrared Spectroscopy and Thermogravimetric analysis. The antibacterial activity of the double layer against the Gram negative Escherichia coli was examined by well disc diffusion method.

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Structural and Optical studies of $Cd_xZn_{1-x}O$ thin films grown by Spray Pyrolysis Technique

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ABSTRACT

Transparent $Cd_xZn_{1-x}O$ thin films of 0.025M concentration were prepared on glass substrate by spray pyrolysis technique. The substrate temperature was fixed at 723K. Deposited films were characterized by X-ray diffractometer (XRD) and UV- visible spectrophotometer. XRD studies revealed that deposited films were polycrystalline in nature and the crystallinity degraded due to the cadmium doping in ZnO. A narrowing of the energy band gap was observed with increasing cadmium content. Refractive index (*n*) and Urbach energy were calculated for different concentration.

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Structural, morphological, optical, electrical and magnetic properties of Mn doped indium oxide films

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ABSTRACT

Indium oxide (In_2O_3) is an important wide-band-gap transparent semiconductor which is widely used as an industrial transparent conducting oxide (TCO) material. Undoped In_2O_3 and Mn doped In_2O_3 films for different Mn doping concentrations viz., 0.5, 1, 2, 3, 5, 7 and 10 wt % are prepared by RF magnetron sputtering technique. The structural, morphological, optical, electrical and magnetic properties of as-deposited Mn doped In_2O_3 films are studied using XRD, micro-Raman, AFM, FESEM, EDS, UV-Visible and photoluminescence (PL) spectroscopy, Hall effect measurement and SQUID magnetometer. XRD patterns show cubic bixbyite structure of In_2O_3 for all the Mn doped films. An enhancement in crystallinity is observed up to 1 wt % Mn doping concentration and there after it decreases. Micro-Raman analysis supports the cubic bixbyite structure of In_2O_3 in the films. The AFM and FESEM images show a uniform and dense distribution of grains in all the films. The films exhibit high transmittance of the order of 78-82 % in the wavelength region 400-900 nm. Intense near band edge UV emission is observed in all the films. Visible emission is shown by doped films with Mn doping concentration in the range 1-10 wt%. Electrical resistivity increases for

the Mn doped In_2O_3 films compared to the undoped film. Magnetic properties of the Mn doped In_2O_3 films are examined.

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Synthesis and structural analysis of perovskite $PbNi_{1/3}Nb_{2/3}O_3$ ceramic

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ABSTRACT

Lead based perovskite ferroelectrics in which B-site is occupied by Ni, Fe or Co, like lead nickel niobate $Pb(Ni_{1/3}Nb_{2/3})O_3$: (PNN), lead iron niobate ($Pb(Fe_{1/3}Nb_{2/3})O_3$: (PFN) lead cobalt niobate ($Pb(Co_{1/3}Nb_{2/3})O_3$: (PCN) are promising multiferroic materials because of possibility having magnetic and ferroelectric order present in the same material. Lead nickel niobate ($Pb(Ni_{1/3}Nb_{2/3})O_3$: (PNN)) is the only known relaxor ferroelectric material in which B-site is occupied by a magnetic transition metal ion and display relaxor like dielectric characteristics. PFN and PCN do not show relaxor like dielectric characteristics because of very high dielectric loss. Relaxor ferroelectrics are very useful in multilayer capacitors, transducers and micro-positioner application because of its high dielectric constant and hystresis free P-E and strain-field curve. Lead based perovskite ferroelectrics are generally very difficult to prepare in single perovskite phase due to volatile nature of lead [1]. The columbite method is generally used to get rid of the secondary (pyrochlore) phase in lead based perovskite oxides. The purpose of this work was to study the role of lead oxide loss in the perovskite phase synthesis of PNN. It is believed that lead oxide loss during calcinations or sintering process leads to the formation of secondary phase. Solid state reaction route and Columbite method are used to synthesis $Pb(Ni_{1/3}Nb_{2/3})O_3$ powder at different calcinations temperatures. Phase analysis reveals the presence of minor peaks corresponds to unreacted PbO and NiO along with lead niobate ($Pb_{1.45}Nb_2O_{6.26}$ - JCPDF-84-1731) and desired perovskite phase in PNN powders synthesized irrespective of the method. The un-reacted powder concentration is reduced with increase of calcinations temperature. The concentration

of second phase, lead niobate, is found ~ 9% and ~ 11% in PNN powder prepared by the solid state route and the Columbite route, respectively. Lead oxide loss during calcination leading to secondary phase is confirmed when single perovskite phase is obtained with 2 wt% excess lead. Rietveld analysis of the X-ray diffraction pattern reveals pseudo cubic structure with Pm-3m symmetry having lattice constant a = 4.0305(2) Å. The quality of fitness parameter (R_p = 5.54, R_{wp} = 6.98, R_{exp} = 3.36, χ^2 = 4.33, R_b = 4.43, R_f = 3.64) agrees well with the literature [2]. Large value of thermal parameters of Pb^{2+} and O^{2-} depicts that these are highly disordered in the lattice. The presence of unreacted PbO and NiO in the powder synthesized by the Columbite method is quite interesting because single phase nickle niobate, $NiNb_2O_6$(NN- JCPDF -72-0481) and lead oxide were starting reagents. Mechanism for the formation of NiO in the calcined PNN powder prepared by the Columbite method will be discussed.

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Eco friendly electrospun polymer coated fertilizers to boost nutrient use efficiency

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ABSTRACT

The fertilizers apart from providing nutrients also get leached into the soil leading to environmental pollution. As a result, the requirement is to have fertilizers which release nutrients at a pace which is equal to the rate of uptake of nutrients by the plants. Electrospinning is a versatile technique which provides such controlled release. Therefore fabrication of control release fertilizers using electrospun polymers and nutrient release study from these nanofibers have been investigated. In this work, the fertilizer namely urea are incorporated in the nanofibers of ethyl cellulose blends, to make controlled release fertilizers. On optimisation a 5% and 10% solution of hydroxy ethyl cellulose (HEC) and Poly vinyl alcohol (PVA) respectively taken in the ratio 1:1(v/v) was found to yield electrospun nanofibers. About 20% of urea (by weight of polymer) was loaded to produce urea incorporated HEC- PVA nanofibers. These fibers were studied by Fourier transform infrared absorption spectra (FTIR) for possible interaction between urea, PVA and HEC. The fibers were further studied by XRD, TGA and SEM analysis. The release of the nutrients was studied using conductivity meter. The pattern of nutrient release was analysed using conductometer. The rate of nutrient release was plotted against the time taken and it was found to follow first order kinetics. Such information are useful in nutrient encapsulation leading to potential improvement in nutrient use efficiency and crop yield.

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Investigation of Third order Nonlinear optical properties and optical limiting studies of (2E,4E)-1-(3-bromophenyl)-5-phenylpenta-2,4-dien-1-one using CW Laser

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ABSTRACT

A new Nonlinear optical material (2E,4E)-1-(3-bromophenyl)-5-phenylpenta-2,4-dien-1-one (known as Ci3BC) has been successfully synthesized and the third order nonlinear optical properties were studied by using Z-scan technique with the help of continuous wave DPSS (diode pumped solid state) laser. The nonlinear optical character was done with the help of UV-Vis spectroscopy which suggests that the synthesized material is transparent at above the cut off wavelength. The Z-scan experiment was performed at 532 nm using DPSS laser having 200 mW output power. Open aperture data gives the 2PA coefficient 0.75×10^{-4}cm/W, whereas the closed aperture data gives the nonlinear refraction coefficient -1.65×10^{-7}cm^2/W. The third order nonlinear optical susceptibility and the second order hyperpolarizability were found to be 1.41×10^{-5} esu and 5.83×10^{-25} esu respectively. Optical limiting studies were carried out by using OA data and hence the limiting threshold was calculated, which is found to be 1.85 KJ/cm^2 for Ci3BC compound. Therefore, the synthesized Ci3BC material has better applications in the optics and photonic devices.

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Investigation of A7 to simple cubic phase transition of arsenic by first principle studies

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ABSTRACT

We report on our investigation of the crystal structure of arsenic under compression, focusing mainly on the pressure-induced A7 → simple cubic (sc) phase transition. The two-atom rhombohedral unit cell is subjected to pressures ranging from 0 GPa to 50 GPa; for each given pressure, cell lengths and angles, as well as atomic positions, are allowed to vary until the fully relaxed structure is obtained. We find that the nearest and next-nearest neighbor distances give the clearest indication of the occurrence of a structural phase transition. Calculations are performed using the local density approximation (LDA) and the PBE and PW91 generalized gradient approximations for the exchange-correlation functional using QUANTUM ESPRESSO. The A7 → sc transition is found to occur at 30GPa-40GPa, no volume discontinuity is observed across the transition in any of the three cases. k-point grids as dense as 8×8×8 enable us to present reliably converged results for the A7 → sc transition of arsenic.

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Structural, Electronic and Dynamical Properties of Tellurium Dioxide (TeO_2) at High pressure: A first Principles Calculations

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ABSTRACT

The present work reveals high pressure structural, electronic and dynamical properties of TeO_2 at ambient and high pressure conditions. The theoretical study using density functional theory has been carried out at high pressure orthorhombic *Cmcm* and *P21a* Phase. The progressive calculations of electronic band-structure of *Cmcm* phase reveals the change of electronic band gap with increasing the pressure and shows the insulator-metal transition at high pressure. The calculated high pressure phonon dispersion curves shows dynamical stability for *P21a* structures though *Cmcm* having imaginary phonon frequencies at high pressure in the Brillouin zone.

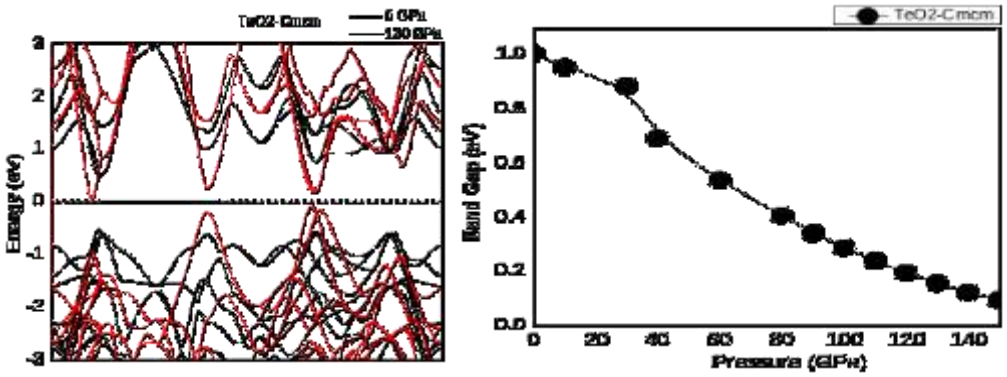

Figure 1(a-b) : Electronic band structure and band gap of TeO_2 of *Cmcm* phase at ambient and 130GPa.

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Synthesis and characterization of phosphate glass thin films on metal substrate

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ABSTRACT

Glass with composition $15BaO\text{-}11Na_2O\text{-}29CaO\text{-}45P_2O_5$ was prepared by melt quenching technique. The density of the glass was measured using Archimedes' principle. The amorphous nature of the prepared glass was verified by X-ray diffraction (XRD).The glass was coated on the Inconel and Stainless Steel substrate by vitreous enamelling method. The crystalline nature of the coating was proved by XRD. The major crystalline phase present in coating was identified using JCPDS data and the uniform distribution of coating was studied by Scanning Electron Microscope (SEM).

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Structural and Electrical Studies of $Eu_{1-x}Sr_xMnO_3$ Manganites

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ABSTRACT

In the present communication, a systematic study of electrical measurement is presented for $Eu_{1-x}Sr_xMnO_3$ compounds ($0.2 \leq x \leq 0.5$). All the samples were prepared using solid state reaction method. The samples were characterized using XRD and SEM. XRD patterns were analyzed using Rietveld method and it is seen that all the compounds are single phased. The samples are crystallized in orthorhombic crystal structure with Pbnm space group. Rietveld analysis of XRD results show the unit volume is decreasing as increasing the concentration of Sr. the SEM results show that grains size is decreasing with increase the concentration of Sr. The electrical resistivity was measured using conventional four probe method. The samples exhibit insulating behavior in the entire temperature range. The electrical conduction mechanism demonstrated that the small polaron hopping (SPH) is model valid in the high temperature regime, whereas in the low temperature regime, the Variable Range Hopping (VRH) Model is valid.

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Structural and Electrical Properties of Sb doped Cu_2SnSe_3: An efficient thermoelectric material

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ABSTRACT

In the present communication, the effect of Sb doping on the electrical properties of Cu_2SnSe_3 was investigated. The $Cu_2Sn_{1-x}Sb_xSe_3$ ($0 \leq x \leq 0.04$) compounds were prepared using solid state synthesis. The room temperature XRD data were recorded for all samples and XRD data were analyzed using Rietveld refinement. The powder X-ray diffraction pattern of all the samples showed a cubic structure (space group). The surface morphology of all samples characterized by SEM. The temperature dependence electrical resistivity (ρ) was measured using four probe method. The electrical resistivity decreased with increase in Sb content up to x = 0.02, then it increased with further increase in x. It is demonstrated that the small polaron hopping (SPH) model is valid for high temperature regime. The measured electrical resistivity data can be satisfactorily described by the variable hopping model (VRH) at low temperatures.

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Influence of Mn doping on structural and optical properties of ZnO thin films synthesized by chemical spray pyrolysis technique

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ABSTRACT

Undoped and Mn doped ZnO thin films with different doping concentration were synthesized by chemical spray pyrolysis method. Films prepared by using Zinc acetate dehydrate and manganese acetate tetrahydrate at 723K substrate temperature. We have studied the structural and optical properties by using X-ray diffraction (XRD), SEM and UV-spectroscopy. The XRD spectra shows that all the samples are hexagonal wurtzite structures. The calculated crystalline size decreases by doping with Mn content. From the optical studies, the transmittance as well as optical band gap in the wavelength range 350-850nm was found to be decreased after doping of Mn.

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Structural and Optical Properties of Europium Doped Zinc Bismuth Borate Glasses

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ABSTRACT

Quaternary europium -doped $10ZnO - 5Na_2CO_3 - xBi_2O_3 - (84\text{-}x)\ B_2O_3 - 1\ Eu_2O_3$ (x = 50, 40, 30, 20, 10) glasses were synthesized by conventional melt quench technique. Amorphous nature of the glass was confirmed by XRD measurement. Density and refractive index of the samples were measured by Archimedes principle and Brewster's angle method respectively. Absorption and photoluminescence spectra of the sample were recorded to evaluate the optical properties of the glasses. Calculated values of Ω_2, Ω_4 Judd –Ofelt intensity parameter were used to predict the lasing properties of the glasses like total radiative life time, branching ratio, emission cross-section and optical gain. Radiative Decay line measurement showed $10ZnO - 5Na_2CO_3 - 10Bi_2O_3 - 74B_2O_3 - 1Eu_2O_3$ has maximum optical gain and hence, it can be used as active medium for lasing or red phosphor material.

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Optical, Thermal, Electrical and Nano structural Study of PVA-PVP doped with SnO_2 Nanoparticals

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ABSTRACT

It is well known that the desire property of a polymer for a particular application can be obtained by doping and blending. In these cases one can also develop new polymeric materials with a wide variety of physical and chemical properties. It is known that the property of the doped polymers mainly depends on the type of the polymer, chemical nature, size of the dopant and the way the dopant interacts with the polymer. Particularly nanoparticles doped polymer has attracted much attention due to the various applications including of sensor properties. Here the combination of inorganic nanoparticles and an organic polymer provides a simple route to stable and processable composite materials, which integrating the promising properties of both components. In the present study n-type semiconductor SnO_2 nanoparticles were synthesized using standard route and the effect of SnO_2 nanoparticle doping on structural, optical, Electrical and thermal properties of the PVA-PVP polymer blend has been investigated using FTIR, UV-Visible and TGA, AC conductivity techniques. Pure and PVA-PVP/SnO_2 nanocomposites were prepared using solution casting technique. The FTIR study confirmed that the SnO_2 nanoparticle interacts with the OH group of PVA-PVP polymer and forms the complex. The presence of these complexes affects the optical, thermal, electrical and structural properties of the composite. The optical study shows the absorption in the UV region and Transparent in the visible region. The variation in electrical conductivity with doping concentration suggests that the

complex formation due to doping affects the conductivity of the composite. The change in the thermal properties was studied using TGA results and the study reflects that the doping also affects the thermal properties of the composite.

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Synthesis of L-Glutamine capped water soluble YVO_4 nanoparticles

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ABSTRACT

Low water solubility, poor biocompatibility and photobleaching are major flaws that compromise the application of most fluorescent nanoparticles. Oleic acid, sophorolipid and polymer capped fluorescent nanoparticles are incompetent due to their weak hydrophilic tale and tedious synthesis procedure. YVO_4 can become more competent fluorescent materials to resolve these problems. Here, we report the synthesis and physicochemical characterization of Glutamine capped YVO_4 nanoparticles. The adopted hydrothermal synthesis procedure rendered YVO_4 nanoparticles with tetragonal crystal structure. The glutamine capping was confirmed by its functional group using FTIR analysis and the absorption spectra of the studied nanoparticles showed UV-Vis band which is attributed to the $^1A_1 \rightarrow {}^1T_2$ electronic transition in the vanadate group.

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Optical properties of chalcone chromophore doped PVA:NaBr polymer films

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ABSTRACT

Chalcone chromophore doped PVA:NaBr (80:20) polymer films were prepared by solution casting method. Different amount of chalcone viz 0.25, 0.5, 0.75, 1.0 wt% were dissolved in PVA: NaBr using N, N, dimethyl formamide (DMF) as solvent. The prepared films were subjected to different characterization techniques such as FTIR, UV Visible, XRD and Fluorescence measurement. It is found that optical properties of doped polymer films enhanced compared with the pure sample. Also it exhibits significant fluorescence yield. Hence these organic chromophore doped polymer films are the good candidate to fabricate optoelectronic devices.

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Synthesis, single crystal growth and characterization of (2E)-3-(4-bromophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one

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ABSTRACT

A halogen substituted chalcone (2E)-3-(4-bromophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (BMC) is synthesized by Claisen-Schmidt condensation reaction. The chalcone formed is purified by repeated recrystallisation using acetone as solvent. Initially, seed crystals of BMC are obtained by slow evaporation of acetone solution. Large size single crystal of dimension 10mm x 6mm x 4mm was grown by slow evaporation solution growth method. The melting point of BMC is found to be 142^{o}C. This high melting point indicates that the chalcone synthesized has high thermal stability. The nonlinear optical second harmonic generation (SHG) efficiency of BMC is 11U (1U=SHG efficiency of urea). The grown single crystal of BMC is characterized by Nuclear Magnetic Resonance spectroscopy, Fourier Transform Infrared Spectroscopy, UV-Visible spectroscopy and powder X-ray diffraction technique. Theoretical calculation of first order hyperpolarizability (β) of BMC in gaseous state was computed using MOPAC-2012 computational software and was found to be 13.29x10^{-30} esu.

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Preparation and characterization of potassium borate glasses with metal oxides

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ABSTRACT

The alkali borate glasses containing $0.05Li_2O$-$0.25K_2O$-$0.60B_2O_3$-.10ZnO and $0.05Li_2O_3$-$0.25K_2O$-$0.60B_2O_3$-(0.10-x) ZnO –xM where (M=Fe, Mn)) and (x=0.001, 0.002, and 0.004) have been prepared by melt quenching method. The samples were prepared at 1050^0C followed by heat treatment at 400^0C for two hours in order to remove the thermal stresses as well as to improve the local order. The structural studies using XRD showed no peaks indicating the glasses to be amorphous in nature. SEM micrographs showed the absence of precipitate indicating the homogeneity of glasses. The physical properties like density and molar volume were measured and compared. UV-Visible spectroscopic studies were done to understand the optical absorption behaviour of the synthesised glasses.

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Structural and electrical properties of Eu doped $La_{0.7-x}A_xSr_{0.3}MnO_3$ manganites

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ABSTRACT

The structural and electrical properties of the Eu doped $La_{0.7-x}A_xSr_{0.3}MnO_3$ manganite samples were prepared using conventional solid state reaction. The crystallographic phase identification of synthesized samples was carried out by X-ray diffraction (XRD). The XRD pattern is analyzed by using rietveld refinement. The XRD results show that all the samples are single phased and crystallized in Rhombohedral crystal structure with R-3c space group. Surface morphology studies were identifying by SEM. The electrical resistivity measurements were done using four probe methods. Electrical resistivity exhibit the Metal-insulator (M-I) transition at low temperature region. The results reveal that M-I transition shift towards the low temperature region when we doped Eu.

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Synthesis, single crystal growth and characterization of a new Chalcone

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ABSTRACT

A new chalcone with molecular formula $C_{21}H_{20}O_4$ has been synthesized by Claisen-Schmidt condensation reaction. The chalcone formed was purified by repeated recrystallization using acetone as solvent. A seed crystal of the chalcone was obtained by slow evaporation method. Large size single crystal of dimension 13mm x 5mm x 1mm was grown by slow evaporation solution growth method. The melting point of the chalcone is found to be 120^{o}C. This high melting point indicates that the chalcone has high thermal stability. The grown single crystal is characterized by Nuclear Magnetic Resonance spectroscopy, Fourier Transform Infrared Spectroscopy, CHNS analysis and TGA-DTA analysis. Theoretical calculation of first order hyperpolarizability (β) and second order hyperpolarizability (γ) of the chalcones was computed using MOPAC-2012 computational software.

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Structural and optical properties of Curcumin- PVA- ZnO composite nano thin films deposited by RF magnetron sputtering

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ABSTRACT

ZnO is a II-VI compound semiconductor with direct band gap of 3.37eV and a large exciton binding energy of 60meV at room temperature. Because of high UV-protection property ZnO is considered as an ideal UV blocker. Curcumin is an active principle of turmeric recognized as an important natural biomaterial which has a wide range of biological importance. It is used as sunscreen agent because of antioxidant property. Curcumin doped PVA (polyvinyl alcohol) is nontoxic and this improves the bioavailability of curcumin. In the present work, ZnO thin films are deposited on curcumin-PVA composites by RF magnetron sputtering at room temperature. These composite nano films will act as promising UV blocking materials. Structural and optical properties of these composite nano films are studied using Fourier transform infrared spectroscopy (FT-IR), Atomic Force Microscopy (AFM), and UV-Visible spectroscopy (UV-Vis). The FT-IR spectra give information about characteristic bands of stretching and bending vibrations of the functional groups formed in composites. Surface morphology of films is studied by AFM. UV-Vis spectra confirm ZnO sputtering enhances absorption intensity of curcumin-PVA composites.