Proceedings of 29th Annual General Meeting of Materials Research Society of India & National Symposium on Advances in Functional and Exotic Materials

EDITOR

S. ARUMUGAM

Organized by
Centre for High Pressure Research
Bharathidasan University
Tiruchirappalli - 620024

IN ASSOCIATION WITH
MATERIALS RESEARCH SOCIETY OF INDIA
(TRICHY CHAPTER)

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Editor
Prof. S. Arumugam

First Print 2018

ISBN: 978-93-87526-16-7 (e-version)

This edition is manufactured to distribute the participants of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials organized by Centre for High Pressure Research, Bharathidasan University, Tiruchirappalli - 620 024 in association with Materials Research Society of India (Trichy Chapter). For the future usage of the material for commercial purpose, authorization from the publisher is essential.

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PREFACE

29^{TH} ANNUAL GENERAL MEETING OF MATERIALS RESEARCH SOCIETY OF INDIA & NATIONAL SYMPOSIUM ON “ADVANCES IN FUNCTIONAL AND EXOTIC MATERIALS” organized by the Centre for High pressure research, Bharathidasan University, Tiruchirappalli – 620 024, India in Association with prestigious Materials Research Society of India (MRSI-Trichy Chapter), will be during 14-16, February 2018. It is with great pleasure we welcome you all, on behalf of the Organizing Committee of National symposium.

We thank our Honourable Vice-Chancellor of Bharathidasan University, **Prof. P. Manisankar** for his encouragement and support to organize this symposium. We are also very grateful to **Prof. G. Gopinath,** Registrar, Bharthidasan University for providing administrative and constant scientific support.

The thematic relevance focused more than 30 topics on theoretical, experimental interdisciplinary and applied aspects of various materials chosen for this symposium with meticulous justification. The topics for the conference are chosen so as to strengthen the binding between Academicians and Industrialists.

The program of the National symposium consists of Eighteen Sessions comprising of plenary lectures, Invited lectures, Medal Lectures, MRSI honour lectures, Best thesis award presentations, contributed poster presentations covering the latest works of the Materials Science community of the country. The symposium registered with 300 abstracts sent by delegates from various countries.

National symposium would become a fertile ground for the exchange of high quality scientific results and ideas by the researchers and scientists from Academia, Industry and Technology. It would certainly create a strong platform for cutting edge research and innovation in technology. Ultimately, it can enlighten the fresh researchers and fetch the craved support and collaborations to those who have been in the field for several decades.

We thank the funding agencies, **Defence Research & Development Organization (DRDO), Council of Scientific & Industrial Research (CSIR), Science & Engineering Research Board (SERB), Indian National Science Academy (INSA), New Delhi, Board of Nuclear Sciences (BRNS), Mumbai, Jawaharlal Nehru Centre Advanced Scientific Research (JNCASR), Bangalore, Bharathidasan University, Tiruchirappalli** for the financial support to organize this symposium.

The venue for the symposium is SRM Hotel, Tiruchirappalli, India. It is elegantly situated on the centre of the city graciously offering the ambience for peaceful, fruitful, untiring and brainy interaction. We welcome you all to participate in the National symposium and make the event a great success.

S. Arumugam
Editor & Convener

Abstracts

Synthesis of Biocompatible Mn-doped TiO_2 hollow Nanospheres

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Abstract:

Among the various inorganic nanomaterials, TiO_2 holds great promise in biomedical applications because of its biological and chemical inertness. However, the hollow TiO_2 nanostructures have not been much explored in biological studies and hence an attempt have been made to synthesize hollow nanospheres of TiO_2 and Mn-doped TiO_2 at room temperature using carbon spheres as sacrificial core templates. The morphology of the synthesized TiO_2 and Mn doped TiO_2 nanostructures were confirmed through SEM and TEM studies while their chemical composition has been ascertained by XRD and XPS studies. Thermal and XRD studies revealed that phase transformation of TiO_2 from anatase to rutile occurred at temperature as low as 550 °C, when the dopant (i.e., Mn) concentration was increased from 1 to 6 mol %. The biocompatibility studies have been carried out through MTT assay that validated their suitability for biomedical applications.

Keywords: Nanospheres; Biocompatibility; Phase transformation; Biomedical application;

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DOI: https://dx.doi.org/10.5281/zenodo.1170834

Crystal Structure of B site Ordered ABiLiTeO$_6$ (A=Ba, Sr) Dielectric Ceramics

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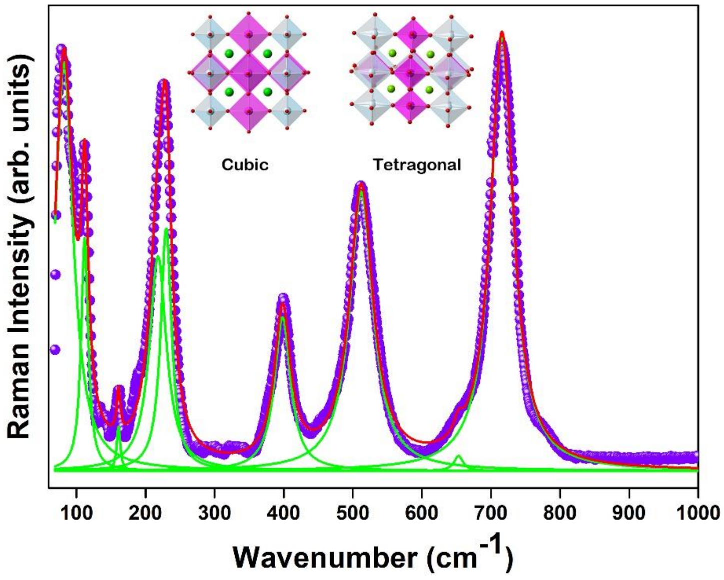
Abstract

Double perovskites are compounds of the type AA'BB'O$_6$ that have been widely studied for their vast structural as well as physical properties. Double perovskites exhibit interesting physical properties and are used as microwave dielectrics, ionic conductors, half metallic conductors, ferroelectrics, superconductors, photo-catalysts and host materials for luminescence centres etc. [1] In the present study, B-site ordered double perovskites ABiLiTeO$_6$ (A=Ba, Sr) were synthesized via solid state reaction route. Even though X-ray diffraction shows a cubic symmetry with space group $Fm\bar{3}m$ a detailed Raman analysis indicates a lower symmetry for all compounds possibly due to tilting of octahedra. The deconvolution of Raman spectra yields more than four Raman active modes which points out a lower symmetry for all these compounds. Fitting of Raman spectra shows number of first order Raman modes is 9 for BaBiLiTeO$_6$ and 7 for SrBiLiTeO$_6$. In accordance with observed number of bands and group theoretical predictions, symmetry of SrBiLiTeO$_6$ and that of BaBiLiTeO$_6$ is tetragonal (I4/m space group). BaBiLiTeO$_6$ and SrBiLiTeO$_6$ possess dielectric constant of 37 and 30 also dielectric loss of 0.028 and 0.024 respectively at 1 MHz.



Deconvoluted Raman spectra for BaBiLiTeO$_6$ ceramics. Experimental data are blue circles while the fitting curve is the red line. Green lines represent the phonon modes adjusted by Lorentzian curves. The cubic and tetragonal double perovskite structures are in inset.

Key words: Double Perovskite, Cation Ordering, Raman Spectra, Dielectric properties

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DOI: https://dx.doi.org/10.5281/zenodo.1170836

Electrical transport properties and applications of some glassy semiconductor

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Abstract

Transition metal oxide (TMO) doped glassy materials generally exhibit semiconducting properties [1, 2]. They are particularly important due to their engrossing applications such as switching, electro–chromatic devices, optical and memory switching devices, etc. [3]. In glasses containing vanadium, the electrical conduction takes place by hopping of unpaired $3d^1$ electron between V^{4+} and V^{5+} states [1, 2]. Frequency and temperature dependent conductivity of TMO doped semiconducting glassy system [4] have been investigated in the wide range of frequency and temperature. The values of activation energy of ac conduction (E_{ac}) and free energy of polaron migration (E_H) [4] have been estimated. Dc conductivity of the as-prepared samples shows thermally activated non–linear nature, which has been interpreted with Vogel–Tamman–Fulcher (VTF) model [4]. Nanostructured glassy semiconductor [5] has been developed as gas sensor, which is strongly related to surface reactions, in terms of change in the concentration of adsorbed oxygen.

Keywords: Transition metal oxide, Ac conductivity, Gas sensor

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DOI: https://dx.doi.org/10.5281/zenodo.1170876

Efficient Green Emission From Ambient Processed All-Inorganic $CsPbBr_2I$ Perovskite Nanorods

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Abstract

The recent renaissance of photovoltaic research has empowered all inorganic perovskite materials to take the center stage thus leading to a plethora of interesting results. Here, a facile room-temperature high quality cesium lead halide perovskite ($CsPbBr_2I$) nanorods has been synthesized. Surface morphology and crystallinity of the synthesized sample were examined by field emission scanning electron microscope (FESEM) and x-ray diffraction (XRD) respectively. For attain further confirmation on crystallinity high resolution transmission electron microscope (TEM) studied was carried out. Elemental composition of the sample was investigated via EDX analysis. These single crystalline nanorods crystallize in orthorhombic phase and exhibit strong photoluminescence emission at 551 nm with narrow FWHM value (~60 meV) and photoluminescence decay time of 22 ns. We believe, this facile synthesis protocol will pave the way for realization other perovskite nanorod and thereby their usage in several optoelectronic arena like as lasing, light emitting diode (1) and photo-detector (2).

Keywords: Perovskites, cesium lead halides, nanorods, photoluminescence

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DOI: https://dx.doi.org/10.5281/zenodo.1170878

Tailoring the topological surface states in $Bi_{1.9}Sb_{0.1}Se_3$by 140 keV proton irradiation

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Abstract

Three-dimensional (3D)topological insulators (TI) are anew class of materials with two-dimensional (2D) conducting Dirac surface states (SS)that host highly mobile and spin-polarized Dirac fermions. Here we report the ion irradiation induced changes in the TI properties.Single crystals of $Bi_{1.9}Sb_{0.1}Se_3$were irradiated with 140 keV proton beam with different ionfluences of 10^{14}, 10^{16}, and 10^{17}ions/cm^2.The magnetotransportstudies on the pristineand proton irradiated $Bi_{1.9}Sb_{0.1}Se_3$ sample shows Subnikov-de Haas (SdH) oscillation and fromLifshitz- Kosovich (LK)analysis, they showed SScharacteristics with Berry phase factor β ~0.6. However, the frequency of theoscillationdecreasessystematicallyfrom 156 T for the pristine sample to 136 T in irradiated sample.From Onsager relation, it depicts that $E_F$is shifteddownward toward the Dirac point (DP). Bulk Carrier density deduced from the Hall data shows a non-monotonicbehavior. Whereas, the surface carrier density deducedfrom the SdHfitexhibits a systematic decrease due to the reductionin the area of the 2DDirac surface states. Proton beaminducedstrain in the sample and its effect on the electronic band structure is believedto shift the Fermi level towards DP. TEM and Raman scattering studies show the existence of compressive strain in the system.

Keywords: **Topological insulators, Ion beam irradiation, Magnetotransport.**

DOI: https://dx.doi.org/10.5281/zenodo.1170884

Fabrication of Porous Alumina Using a Natural Foaming Agent

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Abstract

Porous Alumina was prepared by foaming method using shikakai as natural foaming agent (1). The slurry was gel cast in a plastic moulds. The role of different binders and drying control additives on the porosity development were investigated. Optimization of different process parameters (solid loading, shikakai content and drying temperature) indicated a range of parameters for obtaining strong and porous samples.The nature of the mould influenced the defect in the green cast. It is observed that a flexible and thinner mould was best suited for casting. It is proposed that during the setting of the cast, shape change leads to strain generation and thin wall flexible moulds are the best for obtaining a defect free cast. For every solid loading, an optimum shikakai content is required for obtaining a defect free porous cast. The microstructural features also supported this observation. At higher solid loading, less porous cast was obtained.

Keywords: Alumina, Drying temperature, Drying condition, Moulds, Drainage

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DOI: https://dx.doi.org/10.5281/zenodo.1170890

Shaping Ceramic Cores for Aerospace Application

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Abstract

Demand for higher turbine entry temperature for improved gas turbine efficiency has resulted in design of complex serpentine cooling channels in the castings. The investment casting (IC) process to produce these blades/vanes need cavities of these shapes made of ceramic material. The ceramic cores are of twisted aerofoil shape and have four sections as shown in Fig.1. Shaping ceramic to such complex shapes is possible only through Ceramic injection moulding (CIM). It is a hybrid process having design flexibility of plastic injection molding and diverse material choices from powder metallurgy. CIM process parameters, like holding pressure, melt & mould temperature, cooling time, ejection temperature etc, have associated shrinkage & warpage (S&W) which need to be controlled. Authors have proposed simulation based study to predict, quantify and minimize S&W deviations and defects like weld line, sink marks & air trap. Laser Coordinate measuring machine (CMM) was used to quantify the dimensional deviation in green and sintered ceramic cores as shown in fig.2. Optimisation studies for injection parameters had shown that different set of values are needed to minimise profile or length deviations in the ceramic core.

Keywords: **Ceramic Core, Gas Turbine Blades, Shrinkage & warpage**.

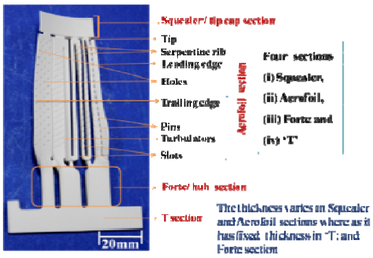

Fig. 1. A typical HPTB core showing different sections

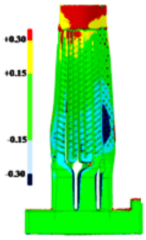

Fig. 2. Dimensional Deviation result from Laser CMM

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DOI: https://dx.doi.org/10.5281/zenodo.1170896

Tuning of Physical and Electrochemical Properties of Nanocrystalline Tungsten Oxide through Ultraviolet Photo activation

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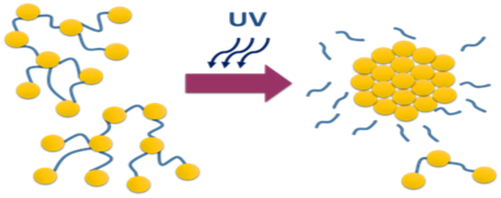
Abstract

In this work, we demonstrate the use of ultraviolet (UV, 365 nm) photoactivation to induce functional changes in the nanocrystalline tungsten oxide (n-WO_3) surfaces. n-WO_3 was initially synthesized by dissolving hydrated-WO_3 powder in 10% H_2O_2 with and without UV exposure. The photoactivation triggered homogeneous ligand-stripping in WO_3 seeds that transformed the random-shaped clusters observed in the unexposed solution into a mono-modal distribution of spherical aggregates. A significant network densification is observed as photo-decomposition of bridging ligands facilitated direct interactions of surface dipoles in those films. We demonstrate that UV-soaking can significantly affect both morphological and chemical parameters such as film compactness, roughness, surface state/trap density and interfacial energy level alignment etc. In the application side, we especially emphasized the electrochromic (EC) and charge storage performances as these are the two most industrially relevant technologies for n-WO_3. A few prototype electrochromic devices (ECDs) and asymmetric capacitors were fabricated using electrodes with and without photoactivation. Both applications showed enhancements in their functionalities owing to the increased number of active sites for electrochemical reactions.



Keywords: **photoactivation, tungsten oxide, impedance spectroscopy, oxygen vacancy**

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DOI: https://dx.doi.org/10.5281/zenodo.1170898

A Study of the thickness and ageing dependent variation in the electrochromic property of V_2O_5 xerogel thin films

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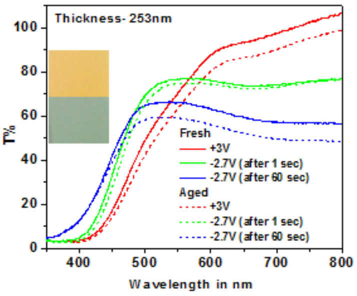
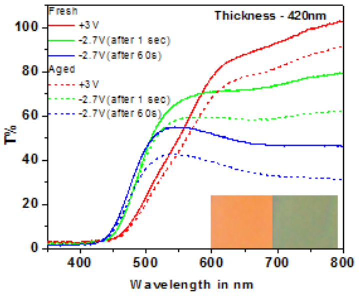
Abstract

Electrochromismis the reversible change in chromic response of materials with electrically concerted charge insertion/extraction. Because of their tenability, the electrochromic materials have widespread applications in the smart windows[1], solar energy modulators[2],display devices[3]and variable emittance surface[4]etc.Among these, V_2O_5 is extensively studied because of their several oxidation states that are adjacent to each other in the energy axes with distinctively different colors. In this work V_2O_5 xerogel thin films of variousthicknesseswere prepared by sol-electrophoresis. With an increase in the film thickness we observed a noticeable decrease in the optical band gap of the material(2.6ev - 2.3ev).The structural and morphological aspects were characterized using XRD, FTIR, SEM and TEMetc. Electrochromic devices (ECD) were fabricated using V_2O_5 xerogel thin films as electroactive layer and electro- opticalresponses were studied using UV-Visible spectroscopy, cyclic voltammetry and chronoamperometry.This study correlates how the ECD performance parameters such as coloration efficiency, color contrast and switching speed is greatly influenced by factors like thickness and ageing.





Keywords - V_2O_5 Xerogel, Electrophoretic deposition, Electrochromic device

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DOI: https://dx.doi.org/10.5281/zenodo.1170900

Synthesis and Characterization of Lanthanum Oxide (La_2o_3) Nanostructures By Using Sol-Gel Method

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ABSTRACT

Lanthanum oxide (La_2O_3) nanostructures were synthesized by a simple sol-gel technique using Lanthanum nitrate, Urea and NaOH starting precursor. The Precursor solution was maintained at 80°C for 6 hours. The samples were washed, dried and calcinated at a temperature of 500°C for 1 hour. The as-prepared and calcinated samples have been subjected to various characterizations The structural and morphological studies of the prepared Lanthanum oxide (La_2O_3) nanoparticles were investigated by means of X-ray diffraction (XRD) and Scanning Electron Microscope (SEM). The X-ray Diffraction (XRD) pattern confirms the formation of Lanthanum oxide (La_2O_3) nanostructures and average size crystallite size was calculated using Debye-Scherrer formula. The prepared samples were subjected to FTIR analysis in order to investigate their vibrational behaviour .

Key words: Lanthanum oxide, Sol-gel technique, Vibrational analysis, SEM.

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DOI: https://dx.doi.org/10.5281/zenodo.1168766

Phase transformation in chemically synthesized Ni nanoparticles

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Abstract

The chemically synthesized Ni nanoparticles exhibit both fcc and hcp structures which are reported to be magnetic and nonmagnetic respectively [1]. Since most of the chemical methods employ carbon-based solvents, the possibility of Ni_3C with crystal structure similar to that of hcp Ni influences the magnetic properties. However, the structure and magnetic property correlation of hcp Ni and Ni_3C are still under debate [2]. Although hcp Ni is ferromagnetic at room temperature from theoretical studies [3], most of the studies report nonmagnetic nature. We show that the nonmagnetic phase is Ni_3C which can be easily identified from the thermomagnetic analysis. The residual magnetism arises due to the presence of trace amount of fcc Ni.

Keywords: Ni_3C, HCP.

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DOI: https://dx.doi.org/10.5281/zenodo.1170936

Facile synthesis of cobalt phosphate as an electrode material for supercapacitor application

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Abstract

The amorphous cobalt phosphates with superior electrochemical performances are achieved via sonochemical method and followed by calcination. The structural crystallinity and surface purity of as synthesized cobalt phosphates are clearly examined via X-ray diffraction and FTIR spectrum. The surface morphology revealed the shape and size of the metal phosphate with respect to sonication process and calcination temperature. The electrochemical studies revealed the maximum specific capacity of 203.4 C/g is achieved with longer cyclic life (92 %) upto 2000 cycles. Therefore, these results conclude that the cobalt phosphate will play a vital role in energy storage application.

Keywords: Cobalt phosphate: Sonication process: Surface morphology: Electrochemical study

DOI: https://dx.doi.org/10.5281/zenodo.1170938

Synthesis and characterization of Ba^{2+} doped $NdCoO_3$ as potential cathode materials for SOFCs application

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Abstract: Solid oxide fuel cells (SOFCs) have attracted great attention in electrochemical devices because of their high energy conversion efficiency, pollution free and widely flexible fuel choices [1, 2]. However, the high operating temperature of about 800 °C - 1000°C leads to technological hurdles in SOFCs technology due to thermal expansion mismatch, chemical reactivity among the components and long term durability [3-5]. These difficulties could be minimized by lowering the operating temperature; nevertheless it reduces the electrode kinetics. Hence, there is a need for the development of alternate cathode materials. The present work aims to develop nanocrystalline Ba^{2+} doped $NdCoO_3$ perovskite oxides materials for ITSOFC applications. Nanocrystalline Ba^{2+} doped $NdCoO_3$ samples were prepared by using combustion process and characterized by XRD, FTIR and SEM-EDX techniques. Further the thermal expansion, chemical compatibility, and electrochemical performance of the prepared Ba^{2+} doped $NdCoO_3$ materials were investigated. Detailed results will be presented and discussed.

Key words: Combustion Process, Perovskite oxides, XRD, SEM-EDX and Electrical conductivity.

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DOI: https://dx.doi.org/10.5281/zenodo.1170940

Temperature and frequency dependence dielectric and complex impedance studies on composite of lead titanate and strontium sexaferrite ($PbTiO_3$ – $SrFe_{12}O_{19}$)

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Abstract.

The work describes the use of dielectric and ac complex impedance spectroscopy techniques to obtain the electrical parameters like electrical conductivity and activation energy of composite multiferroic having composition (x) $PbTiO_3$ – (1-x) $SrFe_{12}O_{19}$; where x = 0.10, 0.30, 0.50 in the frequency range 10 - 1000 KHz over a temperature range of 30 - 550 ^{0}C. The coexistence of low dielectric constant region with high dielectric constant region results in Maxwell – Wagner (M-W) polarization in the composite. Complex impedance spectroscopic analysis indicated the presence of non-Debye type dielectric relaxation in the composites.The grain (R_g) and grain boundary resistance (R_{gb}) decreases with increase in temperature providing convincing evidence that the electrical properties of composite are temperature as well as microstructure dependent. The ac conductivity of composite calculated from dielectric loss and it shows an increase with increasing temperature suggesting semiconductor behavior.

Keywords: Nano composites, dielectric, ceramics.

DOI: https://dx.doi.org/10.5281/zenodo.1170942

Flexible, Conducting Electrospun Pt Nanoislands@Carbon Nanofibers for Low-Temperature H_2 Gas Sensor Applications

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ABSTRACT

Self standing electrospun carbon nanofibers (CNFs) have a lot of applications due to their high surface area, controllable electronic conductivity and simplicity of preparation. Incorporation of catalytic, Platinum nanoparticles (Pt NPs), onto CNFs can enhance their electron transport properties. Herein, we report a two-step process for the successful development of highly flexible and conducting carbon nanofibers with surface anchored Platinum nanoislands (PtNI@CNFs) using a simple combination of electrospinning and electrochemical deposition. Surface morphology of the PtNI@CNFs was characterized using Scanning Electron Microscopy and Atomic force microscopy. Homogeneous distribution of Pt NIs on the surface of CNFs were characterized by HRTEM. Thermal analysis of the material was analyzed using TGA. The coverage density of Pt NIs on the surface of CNFs could be controlled by varying the deposition time during electrochemical deposition. The electron transport properties of CNFs and PtNI@CNFs were studied using I-V measurements. Low temperature H_2 gas sensing properties of CNFs and PtNI@CNFs were analyzed.

Key words: Electrospinning, Electrochemical deposition, Carbon nanofibers, Pt NI@CNF, gas sensors

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DOI: https://dx.doi.org/10.5281/zenodo.1170944

Jamun seed derived activated carbon as an efficient adsorbent for methylene blue removal

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Abstract:

The removal of carcinogenic aqueous pollutants by using activated carbons produced from cheap and renewable precursors such as agricultural wastes has received great attention because of its low cost and high performance. Methylene blue (MB) which is one of the most commonly used cationic dye for coloring, may cause adverse effects to many forms of life [1]. In this study, we have used Jamun seed, an inexpensive biomass as a precursor to prepare activated carbon by chemical activation with KOH, followed by pyrolysis at 900°C [2].This high surface area (747.5 m^2 g^{-1}) possessed activated carbon was used for MB removal from aqueous solution.Batch adsorption studies were conducted under varying conditions of influential parameters and the maximum removal efficiency was found to be 97.77% at room temperature.Experimental data were analyzed using various isotherms and kinetic models followed by the thermodynamic study in order to understand the adsorption mechanism in detail.

Keywords: Jamun seed, Activated carbon, Methylene blue, Adsorption

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DOI: https://dx.doi.org/10.5281/zenodo.1170946

Synthesis of gadolinium doped nickel zinc ferrite nanoparticles for biosensor application

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Abstract

The promising ferrite nanoparticles are now-a-days widely used in the field of biological and medical science due to their high surface-to-volume ratio, superparamagnetic nature and easily tuned by external magnetic field.These magnetic nanoparticles can develop linkages with minute antibiotic-resistant bacteria present in contaminated waste water, for fighting nosocomial infections and in medical field used for MRI, hyperthermia treatment and biosensor applications. Nickel zinc ferrite nanoparticles with composition of $(NiZn)_{0.5}Gd_xFe_2O_4$ (where x=0.1, 0.2, 0.3) were synthesized by economic and facilechemical co-precipitation process. The structure, lattice parameters and crystalline size of these prepared nano particles are derived from their X-ray diffraction patterns to correlate their dependence on gadolinium ions concentration. These random shaped nanoparticles have facetted morphology with sharp edges and vertices as seen from HRTEM micrographs. The average particle size is found to vary from 15 - 25 nm. FTIR transmission spectra of these NiZn ferrite nanoparticlesare recorded in 4000–400 cm^{-1} by using sample in a KBr pellet form. The strong transmittance peaks at about 540 cm^{-1} and 480 cm^{-1} are the characteristic stretching modes arising from the vibrations of FeO_4 tetrahedron and FeO_6 octahedron present in spinel gadolinium ions doped NiZn ferrite nanoparticles. In addition to these modes, the transmission peaks pertaining to the surfactant oleic acidcarbonyl (-COOH), methyl ($-CH_3$), methylene ($-CH_2$), ethene (-CH=CH-) and C-C functional groups are obtained as weak, medium and strong intensity peaks in ~ 1760-1000 cm^{-1} region. The appearance of these peaks confirms the capping of nanoparticles through weak hydrogen bonding. The magnetic measurements are also carried at room temperature by using VSM technique. The saturation magnetization of these samples is found to decrease with increase in gadolinium concentration.

Keywords: Co precipitation, Magnetic, FTIR.

DOI: https://dx.doi.org/10.5281/zenodo.1170948

Morphology and local current mapping of wrinkled reduced graphene oxide

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Abstract

The heterogeneous electronic structure of reduced graphene oxide (rGO) due to the presence of sp^2 and sp^3 bonding make it a promising candidate for many applications including energy storage. However, in order to utilize the material for applications it is essential to understand the nanoscale behavior of the rGO, especially how wrinkling affect the structural and electronic properties. Here, we use a conducting atomic force microscopy (CAFM) to correlate the structural and electrical characteristics of rGO. The rGO wrinkles (~110 nm in width and ~ 8 nm in height) show larger electrical conductance (25 pA) than the other part of rGO sheets (inset Fig.1b). I-V spectroscopy measurement (Fig.1b) further demonstrates that the wrinkles have low turn-on voltage (7.4 V), indicating the electrical conduction occurs through inter–layer tunneling mechanism, which is in agreement with recent predictions [1]. These results emphasize the morphology and electronic properties of wrinkled rGO, which will be useful for graphene based electronic devices.

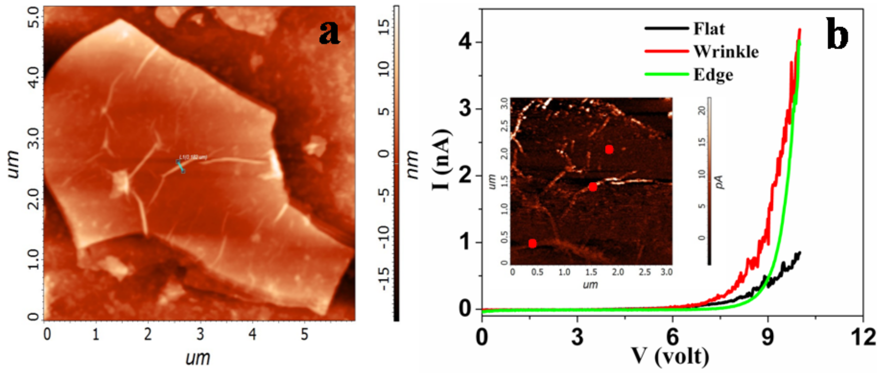

Figure 1. Representative AFM topographic image of rGO (a) and current-voltage measurement of rGO at different regions marked in CAFM image (inset fig.b).

Keywords: Graphene-oxide, current domains, wrinkles and inter-layers tunneling.

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DOI: https://dx.doi.org/10.5281/zenodo.1170950

Valence instability in nano-form of $EuPd_2Si_2$compound

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Abstratct

$EuPd_2Si_2$ is a unique valence fluctuating system which exhibits cooperative and continuous valence transition at about 150K and has been extensively investigated [1]. We have prepared the compound $EuPd_2Si_2$ in nanocrystalline form by high-energyball-milling technique. The compound is found to retain the $ThCr_2Si_2$-type tetragonal structure while the average particle size decreases to less than 10 nm after a milling time of 2.5 hours. We report here detailed investigation of Eu valence state using the microscopic technique of Mössbauer spectroscopy. We find that the Mössbauer spectra of the nanocrystalline compound is divalent like at room temperature and becomes bimodal with lowering temperature unlike that of the parent compound. There is a progressive transfer of intensity from divalent like state to trivalent like state with decreasing temperature. In other words there appears to be a disorder broadened first order valence transition with decreasing temperature unlike for the bulk form. However, the transfer of intensity ceases below about 50K and a significant fractionreveals divalent state for Eu. A clear hyperfine splitting of the divalent component is observed at 4.2K, thereby confirming that the divalent likecomponent ultimately orders magnetically below about 12K. Thus there is a qualitative change in the valence behavior in this compound as the particle size is reduced, which is reported for the first time for Eu based mixed valent compound. There are qualitative changes in the temperature dependent magnetic susceptibility as well.

Keywords :Nanomaterials, Valance fluctuations, Mössbauer spectroscopy

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DOI: https://dx.doi.org/10.5281/zenodo.1170952

Multiferroicity in Haldane chain based polycrystalline R_2BaNiO_5 (R=Tb, Sm)

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Abstract

The rare-earth (R) family, R_2BaNiO_5, crystallizing in an orthorhombic structure (space group: Immm), has been considered to be the first convincing example for Haldane spin-chain behavior and the spinchain anomalies arise from Ni (S = 1). While these compounds attracted considerable attraction over several years from the magnetism point of view, the highly insulating nature of these materials somehow escaped the attention of the community to search for magnetoelectric coupling effects. In the present work we have taken two system R_2BaNiO_5 (R=Tb, Sm) to explore its ferroelectric as well as magneto-electric effects. Tb_2BaNiO_5 has been known to order antiferromagnetically below (T_N =) 63 K. The present magnetic studies on the polycrystals bring out that there is another magnetic transition at a lower temperature (T_2 =) 25 K with pronounced magnetic-field-induced metamagnetic and metaelectricbehaviors. Multiferroic features are found below T_2. The most intriguing observation is that the magneto-dielectric effect is intrinsic and largest (e.g., ∼18% at 15 K) within this Haldane spin-chain family R_2BaNiO_5. Sm_2BaNiO_5, which has been proposed to order antiferromagnetically around (T_N=) 55 K, was investigated for its complex dielectric permittivity, magnetodielectric and pyrocurrent behavior as a function of temperature (T). The pyrocurrent measured in the presence of a bias electric field as well as dielectric constant reveal a weak peak with increasing T around 22 K–the temperature around which population of the exchange-split excited state of Kramers doublet has been known to occur. This finding suggests that this compound presents a novel situation in which multiferroicity is induced by an interplay between crystal-field effects and exchange interaction.

Keywords: Haldane Chain, Multiferroicity, ferroelectric etc.

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DOI: https://dx.doi.org/10.5281/zenodo.1170954

Nanostructured metal oxides as efficient photocatalytic material

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Metal oxides are considered to be promising photocatalystbecause of their efficiency in generation of charge carriers on exposure of light.According to the literature, metal oxides such as TiO_2,ZnO, CeO_2, ZrO_2, WO_3, SnO_2, and α-Fe_2O_3 are proven to be efficientcatalysts in the field of photocatalysis [1],[2]. We are involved in the formation of the faceted structure of ZnO and theirphotocatalytic application.Faceted structures are important as the type of exposed facet have astrong influence on the catalytic activity of the nanomaterials [3].We have synthesized faceted structures of ZnOby the decomposition of zinc oxalate in the presence of flux.Here, we have used NaCl and KCl asflux for preferential growth of (110) plane.We have observed a high value of texture coefficient for(110) plane in the presence of mixture of NaCl-KCl as flux.These faceted structures were used for the photocatalytic degradation of aqueous solution RhB dye. We observed that 53% of the degradation occurred in 70 minutes for ZnO synthesized in the absence of flux whereas ~61% and 63% of the dye was degraded when ZnO formed in presence of NaCl and KClrespectively as a flux were used as photocatalyst.Apart from this,we have carried out photocatalytic activity on various other oxides such as hollow nanostructures of ZnO, $BiFeO_3$, and $ZnFe_2O_4$. We have synthesized hollow ZnO spheres using PEG400 as structure directing agent and carried out its photocatalytic activity.We observed that RhB dye was degraded up to 99% in 50 min on irradiation of ultra-violet light using these hollow spheres.

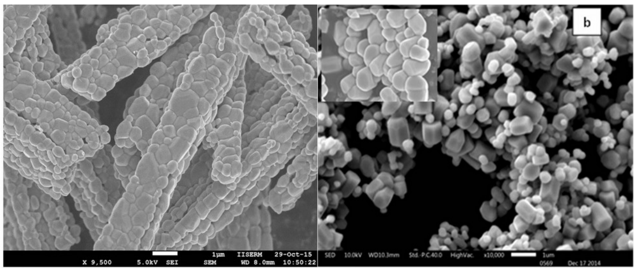

Fig.1 (a) SEM images of ZnO in (a) absence of flux, with (b) 1:1 mixture of NaCl-KCl.

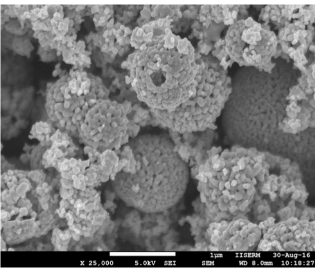

Fig.2 SEM image of ZnO hollow structure.

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DOI: https://dx.doi.org/10.5281/zenodo.1168768

Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials

Inhibition of assimilation of Ti with zirconium based thin films

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Abstract

A serious problem in implant materials, namely assimilation, whereby calcium phosphate precipitates from body fluids overTimetal implants might result in bone re-facture during removal operation of the implanted devices after healing. To control such assimilation, physical vapor deposition of Zr metallic glass (MG)and ZrO_2 on Ti substrates were carried out. The calcium phosphate precipitation was evaluated through immersion test inSBF. The EDAX measurement confirms the absence of Ca on TFMG coated samples with P only was detected and whereas in ZrO_2 films the Ca and P were distributed.In vitro electrochemical corrosion studies indicated that the Zr-based TFMG and ZrO_2coatings sustained in the stimulated body-fluid, exhibiting superior corrosion resistance with a lower corrosion penetration rate and better electrochemical stability than the bare crystalline titanium substrate. The cytotoxicity studies showed the coatings were graded as zero and non-cytotoxic in nature.

Key words: Amorphous materials, Glass, Surface treatments, Physical vapour deposition, Bioactivity.

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DOI: https://dx.doi.org/10.5281/zenodo.1170956

Influence of Al substitution on the crystal structure and dielectric properties of $Sr_3YCo_4O_{10+\delta}$double perovskite

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Abstract

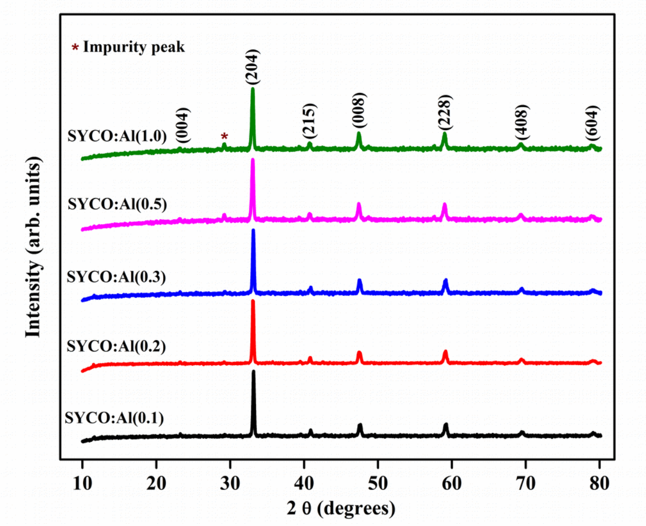

Fig.1. XRD pattern of $Sr_3YCo_{4-x}Al_xO_{10+\delta}$; x = 0.1, 0.2, 0.3, 0.5, 1.0

The complex perovskite related cobalt oxides have recently drawn considerable attention among the scientific community due to their interesting physical properties owing to their multiple valence states (1, 2). In the present study, we investigate the crystal structure and dielectric properties of Al substituted $Sr_3YCo_4O_{10+\delta}$. The Co electronic configuration, primarily determined by the crystalline electric field created by first-neighbor oxygen ions, plays a central role in tuning the electronic properties of this compound. The parent compound under study is ferromagnetic and possesses high dielectric loss. Except ferrites, there are no magneto dielectric materials with low dielectric loss. Hence it would be interesting to tailor the dielectric loss of $Sr_3YCo_4O_{10+\delta}$ by substituting Co sites with Al ions.The compounds were synthesized via conventional solid state ceramic route. A detailed analysis of crystal structure using XRD and Raman spectra will be presented. $Sr_3YCo_4O_{10+\delta}$ crystallize in *I4/mmm* symmetry with lattice parameter of $a = b = 7.642$ Å and $c = 15.342$ Å. On substituting Co site with Al ions, the lattice parameters of the compounds are found to be increasing.The XRD patterns of $Sr_3YCo_{4-x}Al_xO_{10+\delta}$; x = 0.1, 0.2, 0.3, 0.5, 1.0; $\delta \leq 1$ is shown in Fig.1. The microstructure studies were also carried out using SEM. The dielectric properties of $Sr_3YCo_{4-x}Al_xO_{10+\delta}$; x = 0.1,0.2,0.3,0.5,1.0 ; $\delta \leq 1$ were investigated and it was found that the compounds possess a large ε_r value in the order of 10^3 and tan δ of the order of 10^{-1}.

Keywords: Perovskite,Raman spectra, Dielectric properties

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DOI: https://dx.doi.org/10.5281/zenodo.1170958

RGO as active material for electrochemical applications

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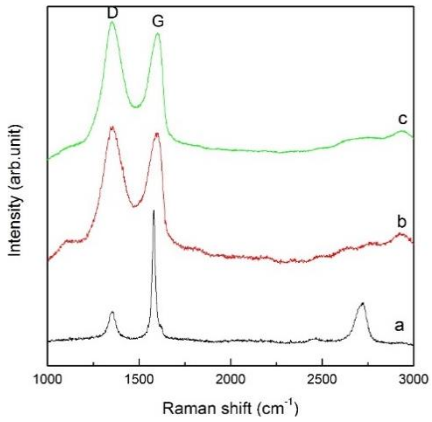
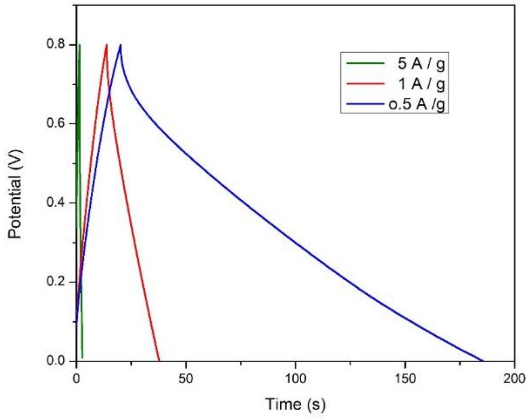
Abstract

Beyond pristine graphene, reduced graphene oxide with a few layers also find important applications in many areas including electrochemical devices. In this context, the reduction of electrically insulating graphite oxide (GO) to reduced graphene oxide (RGO) is important. GO has wide range of oxygen functionalities; the reduction of GO significantly removes these oxygen functional groups. In the present work GO is prepared by modified hummers method and it is reduced using hydrazine [1]. The chemical and structural properties were analyzed by TGA, XRD, SEM and Raman spectroscopy. The structural changes occurred during the transition from GO to RGO is reflected in the Raman spectra. The electrochemical performance of samples were studied using cyclic voltammetry (CV) and galvanostatic charge – discharge (CD) techniques. CD measurements RGO yields a specific capacitance of 232 F/g at 0.5 A/g.





Keywords*: Reduced grphene oxide, modified Hummers method, Specific capacitance*

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DOI: https://dx.doi.org/10.5281/zenodo.1170960

Facile Synthesis and Microwave Absorption Properties of Polypyrrole/$Ba_{0.6}Sr_{0.4}Fe_{12}O_{19}$ Composite in the 8-18 GHz region

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Abstract

The present article reports, synthesis of the Polypyrrole/BSF (PBSF) composite via in-situ polymerization technique and their structural, electrical, magnetic and microwave absorbing properties study in the 8-18 GHz frequency region. The X-ray diffraction patterns reveal the formation of pure hexagonal ferrite phase whereas the Fourier transforms infrared spectrum confirms the formation of polypyrrole/BSF composite structure. The PBSF37 composite shows the highest magnetic moment 59.58 emu/gm rather than the other PBSF composites and pure BSF ferrite also it shows maximum microwave absorption of 89% over the broadband frequency range 8-18 GHz. The maximum shielding effectiveness of 37.49 dB at 15.2 GHz and all other corresponding microwave properties were also studied for the same sample.

Keywords: Composite materials; in-situ polymerization; electromagnetic properties; magnetic moment

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DOI: https://dx.doi.org/10.5281/zenodo.1170962

Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials

Cold Sintering: A Novel Strategy for Densifying Minerals

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Abstract

Cold Sintering (CSP) is a new energy efficient low temperature sintering technique using alkaline or acidic solvents to densify ceramic materials by simultaneously applying temperature (below 300 ^{o}C) and pressure (in MPa range) [1]. The aqueous environment between the ceramic particles enhances densification by a dissolution precipitation process. Since CSP is performed at very low temperatures, the problems due to high temperature sintering such as heat expansion, cracking or dimensional changes of the pellets can be avoided. It has a great potential in integration of ceramics and polymers, silver electrode integration in LTCC, ceramic composites for magnetodielectric applications etc. In the present study, natural garnet mineral, which decomposes above 600 ^{o}C was densified using CSP and the properties were studied. The composites of the garnet with different volume fractions of NaCl (dielectric) and V_2O_5 (conducting) were fabricated using water as the solvent. A pressure of 450 MPa and temperature of 120^{o}C - 200^{o}C was applied for 50 minutes. The composites showed a density in the range of 80 % - 95 %. Crystallographic, microstructural and electrical properties of the composites were studied. For, 0.5 garnet – 0.5 NaCl, dielectric constant (ε_r) = 8.2 & tan δ = 0.02 at f = 10 GHz and for 0.5 garnet-0.5 V_2O_5, ε_r = 240, tan δ = 1.33 & conductivity (σ) = 8.02 × 10^{-3} S/m at f = 1 MHz.

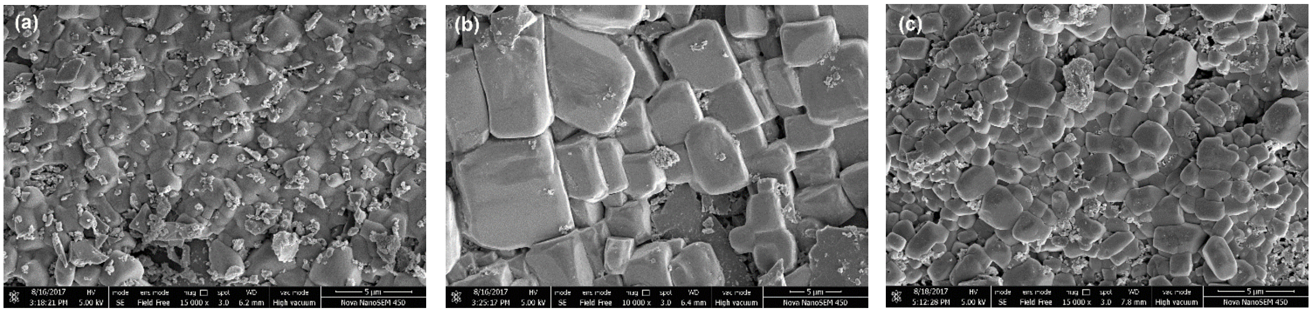

Figure: Microstructure of (1-x) garnet/x NaCl composites (a) x = 0.1 (b) x = 0.3 (c) x = 0.5

Keywords: Cold sintering, Garnet mineral, Microstructure, Electric properties

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DOI: https://dx.doi.org/10.5281/zenodo.1170964

Structural and microwave characterization of $Li_{0.5}Bi_{0.5}MoO_4$in 12-18 GHz regionprepared by solid state reaction method

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Abstract:

In the present work,low temperature firing $Li_{0.5}$ $Bi_{0.5}MoO_4$, has been prepared*via*solid state reaction method and its microwave absorption properties in the 12-18 GHz region have been studied.The Thermogravemetric analysisshowed$Li_{0.5}$ $Bi_{0.5}MoO_4$was thermally stable after 500°C.The structural and microstructural characterizations of the prepared sample were examined through different techniques using XRD, SEM and FTIR spectroscopy. Furthermore, the microwave properties such as reflection loss, shielding effectiveness of the sample were explored in detail. The as synthesized $Li_{0.5}$ $Bi_{0.5}MoO_4$ shows the high reflection loss (RL) value of -35.96dB (>99.9% power absorption) at 14.2 GHz and shielding effectiveness(SE) of-21.83 dB at 13.4 GHz.The RL and SE values observed here are relatively high and could meet the requirement for its use in practical applications.

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DOI: https://dx.doi.org/10.5281/zenodo.1170966

SYNTHESIS GROWTH STRUCTURAL SPECTROSCOPIC AND OPTICAL PROPERTIES OF L-LYSINE SODIUM CHLORIDE NON LINEAR OPTICAL CRYSTALS

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Semi-organic non linear optical material of L-Lysine Sodium chloride was grown by slow evaporation technique at room temperature. Single crystal XRD was carried out to examine the crystal system and unit cell parameters. Powder XRD a pattern confirms the basic structure of materials and the functional groups was identified by using FTIR spectrum. TG/DTA analysis is confirms that the stability of grown crystals. The transparency of grown crystals was analysed by UV-VIS-NIR. The second harmonic generation (SHG) conversion efficiency has been estimated and the output power of the crystal was determined by using Kurtz powder technique.

Key words; Crystal growth;Slow evaporation technique;-Lysine Sodium chloride

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DOI: https://dx.doi.org/10.5281/zenodo.1170968

GROWTH, SPECTROSCOPIC AND OPTICAL STUDIES OF A NEW SEMIORGANIC NONLINEAR OPTICAL CRYSTAL: L-VALINE MAGNESIUM NITRATE

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ABSTRACT

A new semiorganic nonlinear optical crystal, L-Valine Magnesium Nitrate (LVMN), has been synthesized and good optical quality single crystals were grown by slow evaporation technique. The grown crystal was characterized by using FT-IR, UV-vis-NIR and DSC-TGA. The presence of various functional groups was confirmed by FT-IR spectroscopic technique. The UV–vis–NIR spectrum indicates that the crystal has very good absorption in the entire visible and near IR region spectrum suggesting the suitability of the material for NLO applications. The thermal stability of crystal was determined by DSC-TGA studies and mechanical stabilities of crystal have been confirmed by Vicker's microhardness study. The second harmonic generation behavior of LVMN crystal was tested by Kurtz–Perry powder technique.

Keywords: L-Valine Magnesium Nitrate, infrared spectrum, optical transmission spectrum, thermal analysis, and SHG test

DOI: https://dx.doi.org/10.5281/zenodo.1170970

Load Dependent Nanoindentation Studies of Ultrananocrystalline Diamond (UNCD) Thin Films

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Abstract

Ultrananocrystalline diamond (UNCD) films were grown on mirror polished silicon (100) substrates in microwave plasma enhanced chemical vapor deposition system [1]. This film has been attracted widely to scientific community due to its attractive thermal and mechanical properties. Unique mechanical properties of this film was governed by ultranano diamond grains of diamond phase embedded with amorphous carbon (a-C) and short ranged crystalline sp^2 phase [1]. Plastic deformation in UNCD films is mainly located at the grain boundary and dislocation processes within the grain are not active due to ultrasmall size grains [2]. It was shown that the stress required for grain boundary sliding is the main mechanism to determine hardness and yield strength in this material [2]. Our experimental results showed high hardness at lower indentation loads which might be related to strain hardening effect (Fig. 1). This effect has been investigated by high pressure Raman spectroscopic studies on UNCD film which confirmed the hardening upon compression [3]. However, hardness decreased at higher indentation loads, which might be associated to mechanical deformation. Increase in elastic modulus is purely governed by rigid sp^3 bonding of ultranano diamond grains and sp^2 bonding of grain boundary phase. Grain boundaries of UNCD film were found to be highly stable and Raman spectra showed reversible behavior upon release of pressure. This explanation can be considered for improved elastic modulus at higher indentation loads.

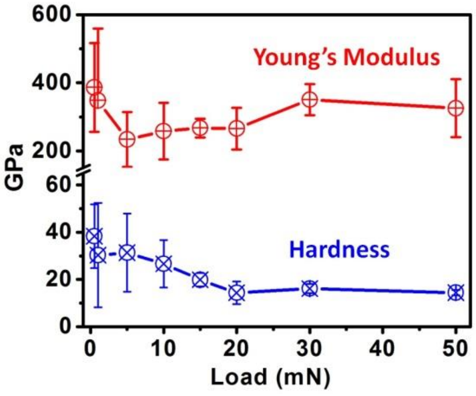

Figure 1. Load dependent nanoindentation study of UNCD film

Keywords

UNCD film, Load dependence, Nanoindentation

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DOI: https://dx.doi.org/10.5281/zenodo.1168770

An Investigation on Photocatalytic and Antibacterial Performance of GO Based Ternary Nanocomposite under Visible Light Irradiation

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Abstract

A facile methodology for the synthesis of novel La_2CuO_4/CeO_2/rGO hybrid nanocomposite was demonstrated via solvothermal assisted homogeneous precipitation method. The phase, crystal structure, surface morphology and elemental composition of synthesized nanocomposite was characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), field emission scanning electron microscopy (FE-SEM), energy dispersive X-ray spectroscopy (EDX) and High resolution transmission electron microscopy (HR-TEM).Absorption range and band gap energy were investigated by UV−Vis diffuse reflectance spectroscopy (UV-Vis DRS). The photocatalytic examination to degrade a target pollutant (Reactive Blue 160) and inactivation of both positive and negative bacterial strains in aqueous solution were investigated under the illumination of visible light. The combination of rGO with binary nanocomposites leads to a better photocatalytic and antibacterial performance than other bare synthesized materials. The enhanced photocatalytic and antibacterial activity of La_2CuO_4/CeO_2/rGO is promising for the further application of visible light driven photocatalyst in polluted water treatment.

Key words: Nanocomposite, rGO - Reduced Graphite oxide, Solvothermal,Photocatalyst, antibacterial activity.

DOI: https://dx.doi.org/10.5281/zenodo.1170972

Influence of Ca, Mn substitution on thermoelectric properties of $SrTiO_3$

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Abstract

Thermoelectric properties have been investigated for $Sr_{0.5}Ca_{0.5}Ti_{1-x}Mn_xO_3$ (x = 0.25, 0.5, 0.75) and $Sr_{0.75}Ca_{0.25}Ti_{0.75}Mn_{0.25}O_3$ polycrystalline samples synthesized by solid-state reaction method. Thermal conductivity, electrical resistivity, seebeck coefficient, power factor and figure of merit (*ZT*) of as prepared samples were studied. The substitution of Ca^{2+} in Sr^{2+} site or/and mixed valence Mnin Ti^{2+} sitecreates appreciable enhancement in the thermoelectric properties and shows increase in thefigure of merit from 0.5 to 0.69 at room temperature. The enrichment of *ZT* around room temperature originates due to low electrical resistivity, low thermal conductivity and high seebeck coefficient of the investigated systems.

Keywords: Thermoelectric, Figure of merit, Power factor, seebeck, electrical resistivity and thermal conductivity, $SrTiO_3$ etc.,

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DOI: https://dx.doi.org/10.5281/zenodo.1170974

Magnetic and Optical properties of mixed oxide $(KNbO_3)_{1-x}+(La_2NiMnO_6)_x$ for photovoltaic application

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Abstract

Multiferroic perovskite oxides $(KNbO_3)_{1-x}+(La_2NiMnO_6)_x$ (x = 0.1, 0.2 and 0.3) with a variation of band gap have been synthesized using the solid-state reaction technique. The structural characterisation of the samples has been carried out by X-ray diffraction (XRD) technique. With the increase of La_2NiMnO_6 (LNMO) percentage in the solid solution, the crystal structure of $KNbO_3$ (KNO) becomes more symmetric from orthorhombic to cubic. Both the XRD and Raman experiment suggest the LNMO concentration dependent phase change in the KNO. The magnetic measurement (Figure) shows the ferromagnetic behaviour of the solid-solution with high Curie temperature (~250 K). Curie temperature, Magnetic moment and saturation magnetisation (at 80 K) increases as the percentage of LMNO in the solid-solution increases. A large reduction in the value of the band gap has been observed in the solid-solution in comparison to the band gap of $KNbO_3$ (~3.6 eV). Photoluminescence (PL) spectra reveals a strong PL quenching in the solid-solutions in comparison to the $KNbO_3$. In respect of the band gap and carrier recombination rate, the solid-solutions show better photovoltaic possibility over $KNbO_3$.

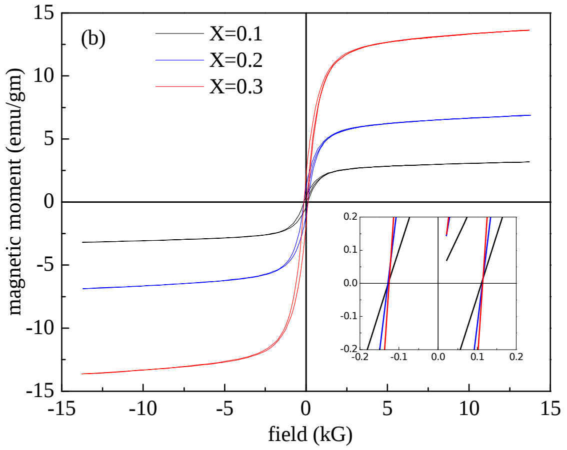

Fig : M-H loop at 80 K of the samples.

DOI: https://dx.doi.org/10.5281/zenodo.1170976

Room temperature ferromagnetism in transparent and conducting Mn-doped SnO_2 thin films

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Tin oxide is an attractive material for solar cells and gas sensing applications due to its high optical transparency (above 80% in the visible range of the electromagnetic spectra) and electrical conductivity (carrier concentration of the order of 10^{20} cm^{-3}) [1, 2]. Recently there is an increased interest to introduce magnetic functionality in tin oxide semiconductors due to their promising applications in spintronics [3, 4]. The tin oxide semiconductor can be made ferromagnetic by doping with transition-metal (TM) ions. The first report of high Curie temperature ferromagnetism in tin oxide thin films was by Ogale et. al. [5], who reported a Curie temperature T_c = 650 K in pulsed laser deposited rutile $(Sn_{1-x}Co_x)O_2$ thin films with x = 5-27%, and an amazingly giant magnetic moment of (7.5+0.5) μ_B per Co ion. The present paper reports the studies on the structural, microstructural, optical and magnetic properties of thin films of $Sn_{1-x}Mn_xO_2$ with molar ratios of x=Mn/(Sn+Mn) = 0.000, 0.025, 0.050, 0.075, 0.100, 0.125 and 0.150, prepared by spray pyrolysis method. The magnetization (M) as a function of magnetic field showed hysteretic behavior at room temperature. According to the temperature dependence of the magnetization, the Curie temperature (T_c) is higher than 350 K. Ferromagnetic Mn-doped tin oxide thin films exhibited low electrical resistivity and high optical transmittance in the visible region (400-800 nm). The coexistence of ferromagnetism, high visible transparency and high electrical conductivity in the Mn-doped SnO_2 films is expected to be a desirable trait for spintronics devices.

Optical transparency; electrical conductivity; ferromagnetism; Curie temperature (T_c); spintronics.

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DOI: https://dx.doi.org/10.5281/zenodo.1170978

Structural/microstructural, magnetic and optical studies on Mn-doped $BiFeO_3$ thin films

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The complex perovskite structures and the most promising magnetoelectric (ME) materials bismuth ferrite $BiFeO_3$ (BFO) have attracted significant attentions over the last few decades due to the coexistence of ferroelectric and antiferromagnetic order at comparatively high transition temperatures $T_C \sim 1125$ K and $T_N \sim 645$ K respectively [1-5]. The paper reports the studies on the structural, microstructural, optical and magnetic properties of $BiFe_{1-x}Mn_xO_3$ with (x = 0.0, 0.02, 0.05) thin films prepared by spray pyrolysis method. The powder x- ray diffraction (PXRD) patterns show a structural phase transformation from rhombohedral structure (**a**=**b**= 5.5694 Å and **c** = 6.8927 Å) with R3m space group for the Mn-doped $BiFe_{1-x}Mn_xO_3$ (x=0.00 & 0.02) thin films to distorted orthorhombic (monoclinic) structure (**a**= 5.79 Å, **b**= 5.6899 Å and **c**= 4.1739 Å) with Cm space group for $BiFe_{1-x}Mn_xO_3$ (x=0.05) thin films. The average crystallite size of $BiFe_{1-x}Mn_xO_3$ was calculated using Debye-Scherrer formula and found to change from 18 nm (x=0) to 43 nm (x=0.05). The microstructural strains calculated from Williamson-Hall plot for the prepared $BiFe_{1-x}Mn_xO_3$ with (x = 0.0, 0.02, 0.05) thin films were found to vary from 0.07576 to 0.00134. The surface morphology of the as prepared films examined by atomic force microscopy (AFM) show that spherical particle (∼100 nm) are densely packed with sharp grain boundary. The local magnetic domain structures of strip-like for the pure and Mn-doped BFO thin film were explored by magnetic force microscopy (MFM). The optical band gap obtained from UV-Vis absorption spectra for the $BiFe_{1-x}Mn_xO_3$ with (x = 0.0, 0.02, 0.05) films were also found to vary in the range of 3.479 eV to 3.386 eV.

Thin films; AFM; MFM; TEM; UV-Vis absorption spectroscopy.

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DOI: https://dx.doi.org/10.5281/zenodo.1170980

Harmonic Generation from Vanillylideneaniline: An Organic Non Linear Optical Material

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NIT, Trichy - 15

Abstract

Single crystals of 2-methoxy-4(phenyliminomethyl)phenol were grown from ethanol by slow evaporation solution growth technique. Crystallization in orthorhombic crystal system with non-centrosymmetric space group $C222_1$ was confirmed by single crystal x-ray diffraction analysis. Preliminary screening of non linear optical activity has been carried out by Kurtz-Perry technique. Computational studies to deduce the favored HOMO-LUMO band gap for non linear optical activity, molecular electrostatic potential and first order hyperpolarizability of the molecule were executed using Gaussian 09 programme. Natural population analysis visualizes the charge distribution in an isolated molecule. By means of measuring third order non linearity using Z-scan, it is proposed that the material can be used for reverse saturable absorption.

Keywords: Crystal growth, Non linear optics, Second harmonic generation, Organic materials,

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DOI: https://dx.doi.org/10.5281/zenodo.1170984

Synthesis of Cu_2znsns_4 thin film by RF-magnetron sputtering for solar cell applications

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Abstract

Polycrystalline Cu_2ZnSnS_4 (CZTS) thin films have been grown on Mo coated glass substrate by RF-magnetron sputtering at substrate temperatures of 573 K, 623 K, 673 K and 723 K. Structural and optical properties of the grown thin films have been investigated by X-ray diffraction (XRD), scanning electron microscope (SEM), Raman spectroscopy and UV-vis spectroscopy. Detailed analysis of XRD data is shown that the grown CZTS thin film has keserite structure (a = 5.4290 and c = 10.849Å) with preferred orientation along (112) plane. All the peaks observed in the XRD pattern have been accounted for kieserite structure, which shows the absence of additional phases such as elemental or binary or ternary systems in the grown film. SEM images recorded with different magnification have showed that the film has smooth and homogeneous surface with average crystallite size 120 nm. Raman spectrum recorded at room temperature which conveys that the dominant Raman shift at 326 cm^{-1} can be attributed to A1 mode and confirms the formation of kieserite CZTS phase. From optical transmittance spectrum, the grown film is found to have direct band gap of ~1.51 eV. The above observations show that the material under investigation is suitable for solar cell application.

Keywords: Cu_2ZnSnS_4; RF magnetron sputtering; Optical band gap.

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DOI: https://dx.doi.org/10.5281/zenodo.1170986

Fabrication of Mg-Zn-Ca metallic glass thinflims by Ion assisted pulsed magnetron sputtering for Biodegradable implants

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Abstract

Ternary Mg–Zn–Ca thin film metallic glasses (TFMG) showed attractive properties making it as potential degradable materials for surface modification of implants, especially compared to traditional crystalline Mg alloys. Mg-Zn-Ca thinfilms of thickness of about 3µm were fabricated using Ion assisted pulsed magnetron sputtering and the amorphous nature of the coatings were confirmed using XRD and TEM-SAED patterns. Nano hardness of 50 Gpa was measured using nanoindendation. In vitro degradation experiments including electrochemical measurements and immersion tests revealed that the zinc could elevate the corrosion potential of Mg in simulated body fluid (SBF) and reduce the degradation rate. As observed from the SEM the coatings were non hemolytic. The cytotoxicity evaluated on L-929 cells revealed that Mg-Zn-Ca TFMG did not induce toxicity in cells.

Keywords: Magnesium metallic glass, Sputtering, Biodegradable, cytotoxicity.

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DOI: https://dx.doi.org/10.5281/zenodo.1170988

Stepwise hydrogelation of a naphthalene diimide appended peptide amphiphile and its application in cell-imaging and intracellular pH sensing

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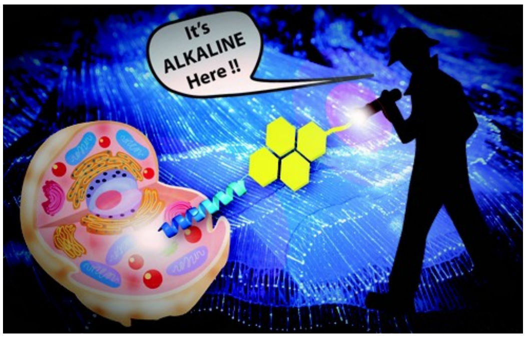
Abstract



This study reports theself-assembly and application of a naphthalene diimide (NDI)-appended peptide amphiphile (PA). H-bonding among the peptide moiety in conjunction with π-stacking between NDI and hydrophobic interactions are the major driving forces behind the stepwise aggregation to form hydrogel. The PA in three self-assembly steps, produced efficient self-assemblies in water at physiological conditions, forming nanofibrous network which further formed self-supportive hydrogel. Importantly, this water soluble conjugate was found to be non-toxic, cell permeable and was used for cell imaging at very low concentration and has an extended biological application to assess intracellular pH.The relatively good biocompatibility and intracellular pH determining capability suggest it as a promising candidate for use as a supramolecular material in biomedical applications.

Hydrogelation, Naphthalene Diimide, Peptide Amphiphile

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DOI: https://dx.doi.org/10.5281/zenodo.1170990

A DNA-NDI hybrid to efficiently detect histone in parts per trillion (ppt) level

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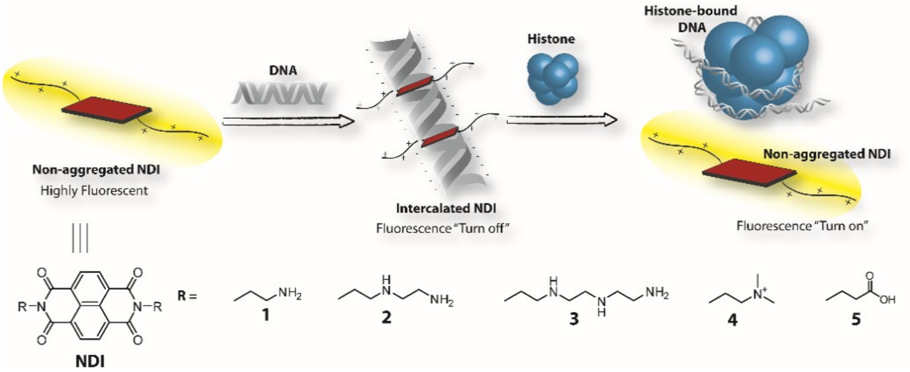
Abstract

Amine and acid functionalized naphthalenediimde (NDI) derivatives were designed and synthesized. The binding affinity of these derivatives were analysed in presence of DNA to identify the most suitable NDI derivative that can be utilized for the detection of histone, a DNA-binding protein.In the monomeric state, the NDI derivatives show high fluorescence but in presence of DNA, the emission quenched. The "turn-off" of emission can be attributed to the formation of NDI-DNA nano-hybrid. Histone, having a stronger binding affinity toward DNA, displaces NDI from DNA. The displacement of NDI leads to fluorescence back to the original monomeric state. So, the quenching of the fluorescence of NDIupon binding with DNA is used to quantitative "turn on" detection of histone with extremely high efficiency and selectivity.



DNA, Histone, Intercalation, Naphthalenediimide, Sensor

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DOI: https://dx.doi.org/10.5281/zenodo.1170992

Tribological Behavior of Ultrananocrystalline Diamond (UNCD) Thin Films by Varying their Growth Conditions

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Abstract: Unique microstructured ultrananocrystalline diamond (UNCD) films are in high demand for several applications including tribology. In this film, wide range of microstructural modifications are possible which tailors the friction and wear properties of films [1,2]. The UNCD films were grown on mirror polished silicon (100) substrates using microwave plasma enhanced chemical vapor deposition system. The deposition was carried out employing either (a) CH_4(1%)/Ar or (b) CH_4(6%)/N_2 plasma media with optimized deposition parameters [1]. Two different microstructures of UNCD films were thus obtained using such a distinct plasma media. Tribological properties of these films were studied considering sliding speed as one of variable parameter. The film deposited in CH_4(1%)/Ar showed friction value in the range of 0.15-0.25. This value was reduced to 0.02-0.1 for film deposited in CH_4(6%)/N_2 plasma media. Low friction in this film was mainly associated to negligible lifetime of run-in behavior. This was explained by large volume fraction of grain boundary which occupies the sp^2 short-range crystalline phase existing with sp^3 bonded ultranano diamond grains [1,2]. Moreover, high wear resistance of these films is inherent property which is related to chemically inert surface. Furthermore, low wear of zirconia ball sliding against CH_4(6%)/N_2 film was related to soft-hard interaction across film-ball contact interfaces [1]. The wear depth of the film was negligible in both the conditions (up to 80 nm) [1,2].

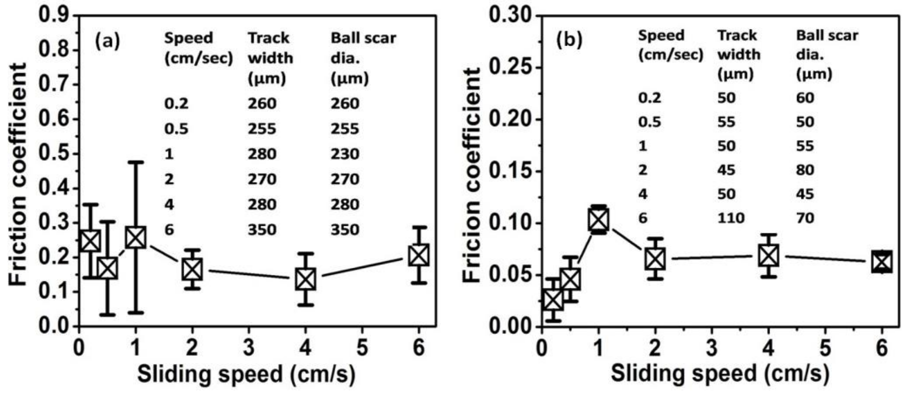

Figure 1. Sliding speed dependent friction behavior in UNCD films deposited in: (a) CH_4 (1%)/Ar and (b) CH_4(6%)/N_2 plasma; Tribology parameters: Ball: ZrO_2 (dia. 6 mm), Load: 2 N, Condition: ambient atmospheric**.** Wear parameters also shown in inset.

Keywords

UNCD film, Sliding speed dependence, Tribological study

Reference

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DOI: https://dx.doi.org/10.5281/zenodo.1168772

Effect of Nickel Substitution on Ammonia Gas Sensing property of Cobalt nano ferrite powders

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Abstract

Atmospheric pollution with toxic gasses is a growing concern. Ferrites in general and nickel ferrite in particular, are reported to be a good sensor for ammonia gas. Here we report a facile and chemical additive-free method to synthesize chromium substituted cobalt nickel ferrite nano-particles (CR-CNFNP) $Co_{0.75}Ni_{0.25}Fe_{2-x}Cr_xO_4$(x=0, 0.20) by auto combustion method. For the as prepared CR-CNFNP ceramic materials, physical and chemical characterization was done by X-ray diffraction (XRD) and energy dispersive spectroscopy (EDS). Diffuse reflectance spectroscopy (DRS) was employed to study the optical band gap values. For sensing study, the high grade aluminum foil strip contacts were used as electrodes for the pelletized CR-CNFNP ceramic material and investigated for ammonia gas sensing response. The room temperature gas sensing studies show that chromium free sample shows increase in sensitivity with increasing ammonia concentration in air and chromium substituted sample shows decrease in sensitivity.

Key Words Spinel ferrite, Sol–gel combustion synthesis, Gas sensor, Nanocrystalas, $Co_{0.75}Ni_{0.25}Fe_2O_4$,chromium substitution

DOI: https://dx.doi.org/10.5281/zenodo.1170994

Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials

Effect of co-polymer on catalytic properties of POMs using one-pot synthesis of Biginelli reaction

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Abstract

Polyether amines belong to a class of green di-block copolymer of ethylene oxide and propylene oxide moieties with terminal amine functionality. These polymers are biocompatible and show temperature dependant phase separation properties. Modification of phosphotungstic acid (PTA) with polyether amine (Jeffamine®) (PTA-Jeffamine®) resulted in a solvent-less liquid-like material. Synthesis of the catalyst (PTA-Jeffamine®) is cost-effective and scalable due to easy availability of the individual components and nature of the synthesis protocol. One-pot synthesis of Biginelli reaction was performed in presence of PTA as catalyst and polyether amine (Jeffamine®) as additive. PTA-Jeffamine simultaneously catalyzes oxidation of benzyl alcohol to benzaldehyde and nucleophilic addition of benzaldehyde, ethyl acetoacetate and urea to form 3, 4-dihydropyrimidinones. Biginelli compounds, 3,4-dihydro-2(1H)-pyrimidinones, are interesting compounds in the fields of therapeutics, synthesis, and bio-organic chemistry. Their derivatives exhibit a wide spectrum of biological effects. The products were characterized by UV-visible, FT-IR, ^{1}H, ^{13}C NMR spectroscopy.

Key words: Polyether amines; catalyst; Biginelli reaction; NMR spectroscopy.

DOI: https://dx.doi.org/10.5281/zenodo.1170996

Structural reconstruction and dual exchange bias in $SrRuO_3/PrMnO_3$ superlattice

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Abstract:

A series of laser ablated superlattice structures with [17-u.c. $SrRuO_3$/n (3,4,5,....,16)-u.c. $PrMnO_3]_{*15}$ have been stacked on (001)-$SrTiO_3$.The refinement of out-of-plane XRD patterns by DIFFaX program ensure the desired artificial fabrication. The Reciprocal Space Mapping (RSM) profiles of the superlattices reveal the stabilization of tetragonal crystal symmetry. The tetragonal symmetry manifests the larger extent of *d-p* orbital overlapping in 180^0 Ru-O-Mn bond, results in stronger interfacial anti-ferromagnetic (AFM) coupling between the spins of Ru and Mn ions[1]. The interplay of AFM coupling energy and Zeeman energy leads to the crossover from negative to positive exchange bias (fig-1) with the increase in cooling field for field cooled field dependent minor loops. The interfacial coupling energy for 5T cooling field was found to be 1.52 erg/cm^2, which is larger compared to those reported for most of the Ferromagnetic/Anti-ferromagnetic systems and 8 times of the coupling energy of $La_{0.7}Sr_{0.3}MnO_3/SrRuO_3$, elucidating the presence of stronger AFM coupling[1].

Keywords: interface engineering, antiferromagnetic coupling, exchange bias

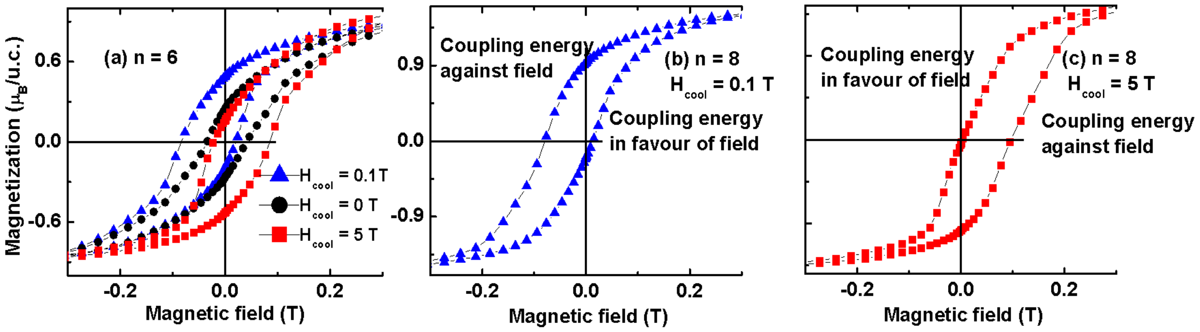

fig-1: Zero-field-cooled, 0.1 and 5 T field−cooled (FC) field-dependent in-plane magnetization at 20 K of (001)STO/[17 u.c. $SrRuO_3$/6 u.c.PrMnO$]_{*15}$ superlattice. (b) 0.1 T and (c) 5 T FC field-dependent in-plane magnetization of (001)STO/[17 u.c. $SrRuO_3$/8 u.c. $PrMnO_3]_{*15}$.

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DOI: https://dx.doi.org/10.5281/zenodo.1170998

Synthesis of porous hollow spheres using aqueous metal ammonium carbonate complex solution as novel precursor for energy storage application

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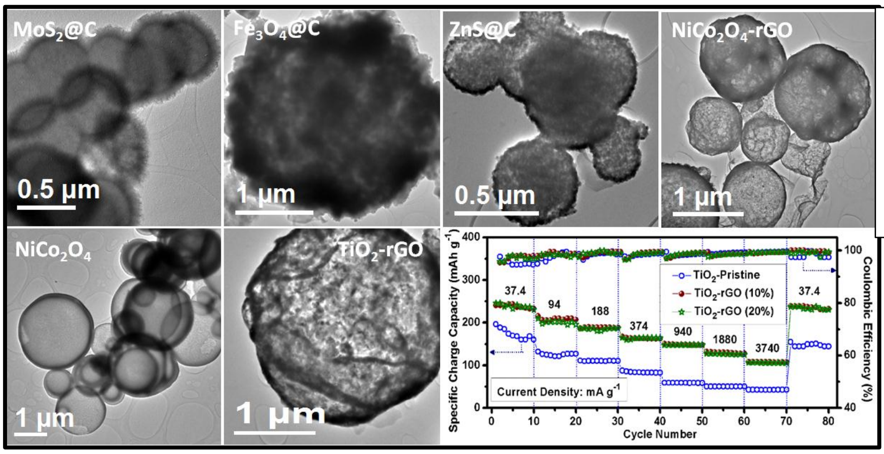
We have developed two simple synthetic strategies for variety of metal oxide/sulfide/carbide and corresponding carbon/rGO incorporated hollow spheres. Different carbon incorporated nanocomposite hollow spheres have been realized using corresponding aqueous metal ammonium carbonate complex solution as precursor, thiourea as sulfur source and combined sucrose-CTAB as simple soft template as well as carbon source through hydrothermal treatment followed by calcination (1-2). In another strategy, pristine and rGO incorporated hollow spheres have also been synthesized through as simple spray-drying based strategy using the identical metal and sulfur precursor without any organic additives (3-4). Synthesized hollow spheres exhibit superior energy storage material as anode in LIB/ECC or active catalyst for H_2 generation through electrochemical water splitting. As for example, TiO_2-rGO (20%) hollow sphere showed exceptionally high capacity of 274 mA h g^{-1} at 18.8 mA g^{-1}.



TEM images of some of the synthesized hollow spheres and corresponding Rate performance of TiO_2 based hollow spheres

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DOI: https://dx.doi.org/10.5281/zenodo.1171000

Cold sintered PVDF polymer – $Ba_{1-x}Sr_xTiO_3$ based ceramic nanocomposites for high energy storage application

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Abstract:

The objective of current work is to study the ferroelectric ceramic $Ba_{0.7}Sr_{0.3}TiO_3$ (BST) –PVDF (Polyvinylidene fluoride) Polymer nanocomposites for energy storage applications. Fairly dense composites have been synthesized using recently invented cold sintering process (CSP) (1, 2) and their dielectric and energy storage properties have been investigated. CSP is a new sintering technique to achieve dense ceramics at extraordinary low temperature ($<200^0$C), providing opportunity to fabricate high content ceramic nanocomposites with polymer reinforcements. Dense samples of BST-PVDF nanocomposites have been prepared below 180°C (at low temperature) with 80% ceramic as a matrix and 20% PVDF as Nano fillers. XRD analysis has been performed. High resolution SEM analysis has been performed which confirms the formation of PVDF coated BST ceramic grains. Energy storage capacity has been qualitatively analysed using P – E hysteresis curves.

Keywords: Cold Sintering, Ferroelectric, Nanocomposites.

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DOI: https://dx.doi.org/10.5281/zenodo.1171002

Deposition of Vanadium Oxide (VO_x) Thin Films by DC and RF Magnetron Sputtering.

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Abstract:

Vanadium oxides represent an important class of materials with high potential in many technological applications based on their diverse temperature-dependent electronic properties. There are large variety of the vanadium oxide phases such as VO, V_2O_3, VO_2, V_2O_5 etc. Depending on the ambient conditions and temperature, phase transformations between these oxides can occur. In addition, several vanadium oxides undergo metal-to-insulator transitions (MIT), e.g., V_2O_3 at ~150 K, VO_2 at ~340 K (67 °C). These complex structural and electronic transformations may play a crucial role in the behavior of vanadium-based systems. Among all, VO_2 has smaller absorption in the far IR wavelength of 8–12 µm and it shows a large temperature coefficient of resistance. VOx thin films were deposited on Si_3N_4/Si(100) substrate by using DC and RF sputtering. The depositions of VOx thin films were carried out by varying substrate temperature, plasma power, Ar/O2 ratio and working pressure. The structural characterization of the films was carried out by using XRD and AFM. The transition temperature of the grown VO_2 thin films was found to be around 65 °C.

Keywords: Vanadium oxide, Sputtering, XRD, AFM

DOI: https://dx.doi.org/10.5281/zenodo.1171004

Highly Sensitive Urea Sensor Based on Citric acid Capped plasmonic Copper quantum dots

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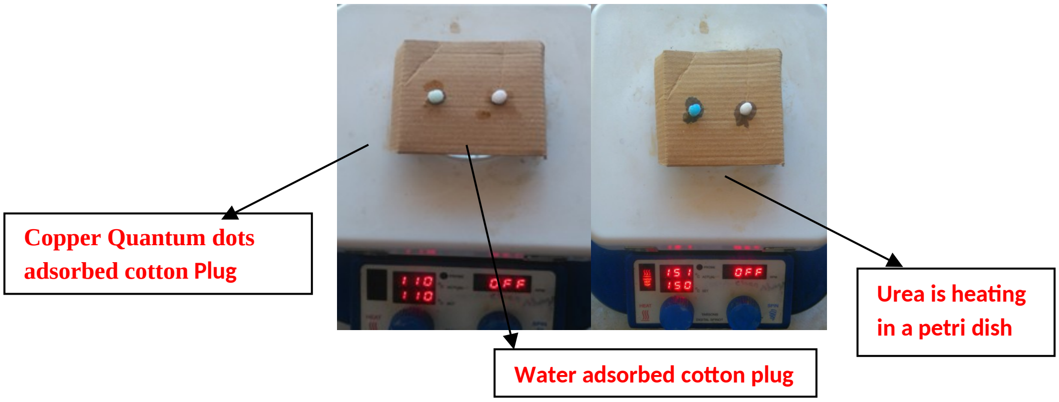
Abstract

Metallic quantum dots have received greater attention due to their wide applications as a colorimetric sensor due to their high sensitivity and easy device integration. Herein, we report a one step method to synthesis metallic copper (CuQDs) quantum dots using citric acid and Sodium Borohydride ($NaBH_4$) as capping and reducing agent, respectively. As prepared CuQDs solution appears light bluish green color due to the Surface Plasmon Resonance (SPR). The color of the CuQDs adsorbed cotton plug changed from light green to dark blue in the presence of Urea. The proposed method can find extensive applications in clinical sensors and also for detecting urea in water samples in high fidelity.



Keywords: Copper Nanoparticles, Surface Plasmon Resonance, Urea.

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DOI: https://dx.doi.org/10.5281/zenodo.1171006

A new emerging ecofriendly rare earth free 2D luminescent nanoprobes for high-contrast *in vitro* and *in vivo* imaging applications

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Abstract

A new emerging ecofriendly rare-earth free, highly luminescent and biocompatible two dimensional (2D) carbon based boron oxynitride (BCNO) was synthesized using facile auto-combustion methodwhich can be easily scaled-up for large quantities. [1] The BCNO exhibits a single, distinct and broad photoluminescence (PL) emission which can be easily tuned from violet to deep red (342 nm to 654 nm) by varying the amount of boron/carbon content. Moreover, time resolved photoluminescence (TRPL) reveals that 2D BCNO have PL lifetime in range of nanosecond. PL and TRPL results indicate that B-O act as luminescence centers, which are responsible for the tunable luminescent properties while carbon impurity induce energy levels in the band gap of 2D BCNO nanophosphors. These tunable and biocompatible luminescent 2D BCNO nanophosphors are potentially used for *in vitro* high-contrast cellular imaging as well as *in vivo* imaging applications.

Keywords: BCNO, photoluminescence, time resolved photoluminescence, *in vitro,in vivo.*

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DOI: https://dx.doi.org/10.5281/zenodo.1168774

"A DFT Study on the Structural and Intermolecular Interaction of Corylin and Daidzein in Neuraminidase receptor"

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ABSTRACT

The successful practice of medicinal chemistry crucially depending upon the understanding of the principles of protein-ligand interactions. Importantly, the polar, hydrophobic and hydrogen bonding interactions are the most probable type of interactions exist between the protein-ligand complexes. In the present study, a theoretical analysis of Corylin and Daidzein molecule was performed from the wave function obtained from the HF and DFT methods with the basis set 6-311G**. The molecular geometric parameters were predicted by DFT method, which are found to be slightly higher than the HF method and the gas phase is compared with active site. A molecular docking and HOMO-LUMO have been carried out to understand the conformational change in the active site of Neuraminidase Receptor. The nearest neighbours, shortest intermolecular contacts between Corylin and Daidzein - Neuraminidase Receptor and the lowest binding energy of Corylin and Daidzein have been analyzed from the docking analysis.

Further, the electrostatic properties of the molecules also determined. The electrostatic potential (ESP) map of the molecules allows identifying the nucleophilic and electrophilic regions of the molecule. The molecular orbital contributions were studied by using the total (TDOS), partial (PDOS), and overlap population (OPDOS) density of states. The theoretical harmonic vibrational frequencies and scaled values were calculated and compared with experimental Fourier Transform infrared (FT-IR) and Fourier Transform Raman (FT-Raman) spectra.

DOI: https://dx.doi.org/10.5281/zenodo.1169021

Influence of Structural Transition on Dielectric and PE measurements of La doped Bismuth Titanate Polycrystals

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Abstract

Pure and La doped bismuth titanate $Bi_{4-x}La_xTi_3O_{12}$ (x=0, 0.15, 0.25, 0.5, 1) polycrystals were prepared by sol-gel process. The crystalline behaviours of all prepared powders were studied by X-ray diffraction analysis (XRD), and the phases were confirmed with JCPDS data. As the La-concentration increases, the shifting of XRD peaks and also merging of certain peaks were observed related to a possible structure change from orthorhombic to tetragonal [1]. This suggested the high centre of symmetry for La doped sample. Differential thermal analysis has been employed to determine the glass transition temperature. DTA measurements were recorded in the temperature range 300^{o} to 800^{o} C, and the phase transition ferro- to para- electric transition has been observed [2]. The value of dielectric constant were decreased with increasing the frequency. Also Ferroelectric loops were obtained for the BT and BLT powders at room temperature. So, the dielectric constant decreases with increasing frequency as well as value of dielectric constant is increased by increasing La concentration [3]. From DTA analysis the Curie temperature is found to lower values by increasing La concentration. Also Hysteresis loops were obtained for both pure and La doped systems, but by La concentration increasing, the space charge polarization cannot keep up with change of electric field, so that the remnant polarization and coercive field decrease.

Keywords: Bismuth Titanates, Doping Effect, Structural Transition, ferro- to para- electric transition

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DOI: https://dx.doi.org/10.5281/zenodo.1169025

Bifunctional anatase TiO_2 thin films for electrochromic and room temperature gas sensing applications

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Abstract. TiO_2 thin films possessing multifunctional properties have application in broad range of spectrum such as dye sensitized solar cells, electrochromic windows, catalysis, gas sensors and lithium ion batteries. Chemical deposition techniques like spin coating; spray deposition and electrodeposition are receiving much attention because of their cost effective, ease in synthesis process. Among these techniques, spray deposition is suitable for large area deposition of transition metal oxide thin films. Anatase TiO_2 film is prepared by nebulized spray deposition technique using isopropanol as a solvent at a low substrate temperature of 200°C. The XRD and Raman studies indicated the formation of anatase TiO_2. Formation of homogeneously distributed pyramidal shaped nanograins was observed from the FESEM study. The electrochromic response of anatase TiO_2 film was studied by intercalating/deintercalating Li^+ ions from 1 M $LiClO_4$ in propylene carbonate solution. TiO_2 films possess excellent electrochromic behavior with excellent coloration efficiency of 157 $cm^2\ C^{-1}$, and a high reversibility of 92%. The TiO_2 thin films were further investigated for gas sensor applications. The TiO_2 thin films showed excellent response for ammonia gas detection as low as 5ppm at room temperature operating condition. The present report suggests that the nebulized spray deposited TiO_2 thin films can perform efficiently for electrochromic and gas sensing applications.

Keywords: TiO_2, Electrochromism, Gas sensor

DOI: https://dx.doi.org/10.5281/zenodo.1169031

Facile synthesis of a novel Ternary Hybrid Hetero junction Photocatalyst (g-C_3N_4/CuO-ZnO) for Water splitting Hydrogen production Applications.

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Abstract

The utilization of solar energy for water splitting paves a way for environmentally friendly H_2 generation.The synthesis of g-C_3N_4 and CuO-ZnO powders was achieved using a conventional pyrolysis and co-precipitation method, respectively. A novel ternary hybrid hetero-junction photocatalyst g-C_3N_4/CuO-ZnO was subsequently prepared through grinding and sonication. The structures, morphologies and optical properties of the photocatalysts were comprehensively characterized and compared with those of g-C3N4. X-ray diffraction results revealed that the g-C3N4/CuO-ZnO sample has well crystalize structure. Spectroscopic results obtained via FT-IR technique were consistent with the layered structure of sp^2 hybridized bonding features of C and N in g-C_3N_4 besides Cu-O, Zn-O stretching vibrations. Photoluminescence results revealed that CuO-ZnO hybridization with g-C_3N_4 showed efficient separation and delayed recombination of photoinduced electron-hole pairs. Microscopy analysis clearly displayed that CuO-ZnO nanoparticles are anchored on g-C_3N_4 and showed the interface between the CuO- ZnO and g-C3N4. The g-C3N4 /CuO-ZnO nanocomposites exhibited enhanced visible light photocatalytic H_2 production.

Keywords : Ternary hybrid, heterojunction, Hydrogen production

DOI: https://dx.doi.org/10.5281/zenodo.1169039

CuO nano flowers – Synthesis and gas sensor application

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Abstract

Air pollution is a growing problem these days. Gas sensors that can identify volatile organic gases (VOCs) or toxic gases are of great importance. Recently, researchers have developed various kinds of gas sensors, such as oxide semiconductors, organic semiconductors, field effect sensors and surface acoustic wave sensors [1,2]. From among the above varieties, oxide semiconductor gas sensors have attracted much attention because of their high sensitivity, low manufacturing cost and simple means of measurement and signal conditioning. Cupric oxide (CuO) is one of the most important p-type oxide semiconductors as it exhibits a stable narrow band gap (1.2–1.9 eV).A simple wet chemical route has been developed for synthesizing cupric oxide (CuO) nanoflowers with excellent reproducibility followed by their utilization in a gas sensor. Copper foil, ammonium persulphate and sodium hydroxide were used as copper precursor, structure directing agent and accelerator, respectively. Characterization studies including x-ray diffraction spectroscopy (XRD), Fourier transform infrared spectroscopy (FTIR), field emission scanning electron microscopy (FESEM), and transmission electron microscopy (TEM) were performed to investigate the structure and morphology of the as-synthesized CuO. At the operating temperature of 240 °C, the response/recovery time of the synthesized sensor was measured for acetone. The fabricatedCuOnanoflower gas sensor responded very prominently for acetone concentrations of 250 ppm and 2250 ppm and the recorded response was 2.7 and 7.2 respectively. The developed method is a low cost, environmentally friendly and fast route to produce high quality CuOnanoflower gas sensors for VOC's detection.

Keywords: Nanoflower; Oxides semiconductor; Gas sensor; Response/Recovery time

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DOI: https://dx.doi.org/10.5281/zenodo.1169085

Superconductivity induced by external pressure in $Eu_{3-x}Sr_xBi_2S_4F_4$ (x=1,2) compounds

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Abstract:

The interplay between superconductivity and Eu^{2+} magnetic ordering in BiS_2 based $Eu_2SrBi_2S_4F_4$ is studied by means of electrical transport and magnetic measurements under external hydrostatic pressure. The parent $Eu_3Bi_2S_4F_4$ (Eu-3244) which shows superconductivity at 1.5 K [1] is different from other BiS_2 superconductors in that they are intrinsic superconductors; namely, no external doping is required to induce superconductivity. The effect of Sr-doping in Eu sites, T_c gradually decreases from 1.5 K to 0.48 K (Sr=1) and there is no sign of SC can be detected further increasing Sr content at x=2 [2,3]. The decreased Eu^{3+} population, and the corresponding lower charge carrier density, may be the main origin for the suppression of superconductivity. We have studied the temperature-pressure phase diagram of two materials $Eu_{3-x}Sr_x Bi_2S_4F_4$ (x = 1 and x = 2) by electrical resistivity and magnetic measurements down to 2 K. Semiconducting resistive behavior observed in both the materials under ambient conditions transforms into metallic behavior as externally applied pressure gradually increases. Superconductivity is observed in both the materials at and above applied pressure P = 2.37 GPa. Under the highest pressure P ~ 2.9 GPa applied in our measurements, T_c is ~ 9.8 K in $Eu_2SrBi_2S_4F_4$ (x = 1) and 8.2 K in $EuSr_2Bi_2S_4F_4$ (x = 2). Upper critical field $H_{c2}(0)$ ~ 3.04 T (x = 1) and 1.17 T (x = 2) is estimated from magnetic field dependent resistivity measurements at 2.9 GPa. Using the Arrhenius equation, we estimate the thermally activated flux flow (TAFF) activation energy U_0 as 116 K in $Eu_2SrBi_2S_4F_4$ and 39 K in $EuSr_2Bi_2S_4F_4$. At 2 K, DC magnetic susceptibility measurements indicate S-type paramagnetic behavior. Our work gives commonality of pressure effect on bismuth oxysulfide based superconductors and also it's uncovers the significance of electron carrier density in the high-T_c superconducting phase.

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DOI: https://dx.doi.org/10.5281/zenodo.1164576

Molybdenum Trioxide Surface Functionalized with Ruthenium(II) and Chitosan: Bio-functional Nanosystem

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Abstract

Environment-friendly approach for large-scale preparation of biomolecule functionalized metal oxide nanostructures are beneficial for fundamental and advanced health care applications [1,2]. Herein, molybdenum trioxide nanoparticles (MoO_3 NPs) are synthesized using asafoetida resin (natural product) as reducing agent and sequentially surface modified with ruthenium(II) [Ru(II)] and biomolecule, chitosan at room temperature. MoO_3 NPs were electrostatically modified with ruthenium(II) resulting into an optically active nanodispersion, exhibiting UV-vis absorbance at 216, 290 and 486 nm, respectively. Spectroscopic investigations revealed that the functional group of $Mo\text{-}O\text{-}Mo^+$ and $Mo{=}O^-$ mediated a cationic-π and anionic-π interactions with bipyridine ligands of Ru(II). Intermolecular interaction with the amine groups of chitosan have established a coordination bonding in MoO_3-Ru(II). It is expected that the chitosan layer modified on the surface of MoO_3-Ru(II) may promote biocompatibility suitable for bio-imaging and biosensor platform.

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DOI: https://dx.doi.org/10.5281/zenodo.1169091

Synthesis, Crystal Growth and Characterization of Cu (II) Doped 4 - bromo - 4′ - hydroxybenzylidene aniline Nonlinear Optical Material

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Abstract

One of the novel benzylidene aniline derivatives, Cu (II) doped 4-bromo- 4′-hydroxybenzylidene aniline (CBHBA) was synthesized and single crystal of CBHBA was grown from solution following slow evaporation method at room temperature. Unit cell parameters of the grown crystal were determined from single crystal X-ray diffraction studies. Functional groups of CBHBA were identified from Fourier Transform Infrared spectral study. UV- Vis - NIR analysis of CBHBA showed that the crystal is transparent between wavelengths 400 and 1100 nm. Thermal stability of the title compound was examined by thermogravimertic and differential scanning calorimetric studies. Fluorescence spectrum of the grown crystal recorded using spectrofluorometer shows emission peak at 450 nm. The second harmonic generation efficiency of CBHBA estimated by Nd:YAG pulsed laser employing the Kurtz powder technique is ~ 1.3 times that of potassium dihydrogen orthophosphate.

Keywords: Organic compounds; Crystal growth; Fourier Transform Infrared Spectroscopy; Thermogravimetric analysis.

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DOI: https://dx.doi.org/10.5281/zenodo.1169097

Synthesis, Growth and Characterization of Zinc Doped Nonlinear Optical Material of 4 - methoxy - 4′- dimethylamino benzylidene aniline

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Abstract

In recent years the interest in synthesizing of organic and semi organic materials with charge correlated and highly delocalized π-electron states and growing them as single crystals has increased considerably, since very large nonlinear optical susceptibilities have been measured in some of the materials to utilize them for various applications. Synthesis, growth and characterization of a novel third order nonlinear optical material, 4-methoxy-4′-dimethylamino benzylidene aniline doped with zinc are reported for the first time. The structural perfection of the grown crystal is analyzed by X-ray diffraction. The functional groups present in the synthesized material are investigated by FTIR and FT-Raman spectral analyses. The placement of the protons is determined using HNMR spectrum. The range and percentage of optical transmission were ascertained by recording UV–VIS–NIR spectrum. Thermal and mechanical properties are also studied. Dielectric study shows that the dielectric constant of the crystal varies with frequency and temperature. The third order nonlinear optical absorption coefficient of the crystal is determined by the Z-scan technique.

Keywords: Organic Compounds, Crystal Growth, Dielectric Studies.

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DOI: https://dx.doi.org/10.5281/zenodo.1169101

Growth and Characterization of Non linear Lithium Sulphate Doped 8-Hydroxyquinoline Single Crystal

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Abstract

In the recent years, numerous research activities have been in progress on non linear optical crystals owing to their key functions in optical modulation, optical switching, frequency doubling and optical memory. The present work deals with the crystal growth of lithium sulphate doped with 8-hydroxyquinoline by slow evaporation solution growth method. The grown crystals are characterized by structural, optical, spectral, mechanical, dielectric and thermal studies. The lattice parameters and crystal structure of the grown crystals are measured by single crystal X-ray diffraction. The presence of functional groups in the grown compound has been confirmed by FTIR technique. The suitability of the grown materials for optical application was studied by using UV-Visible spectroscopy. The second harmonic generation efficiency of grown crystals were recorded by Kurtz and Perry technique with Nd:YAG laser using KDP as a standard material. The hardness of the grown crystal was measured by using Vicker's microhardness tester. To analyze the electrical properties, dielectric constant, dielectric loss and a.c. conductivity of the grown compound were calculated from the frequency range 50 Hz – 5 MHz at different temperatures. The melting point and decomposition of the grown material were investigated using thermo gravimetric and differential thermal analyses studies.

Keywords: NLO Material, Crystal Growth, FTIR, Thermal Analysis.

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DOI: https://dx.doi.org/

Comparative Study of Nonlinear Optical Properties of Benzylidene Aniline Derivatives

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Abstract

Nonlinear optical materials have recently attracted much attention because of their potential applications in emerging technologies like signal transmission, data storage, optical switching, laser printing, displays, photolithography, remote sensing, chemical and biological species detection, high resolution spectroscopy, medical diagnosis and under water monitoring and communication. Some polar organic crystals, which form a non-centrosymmetric structure exhibit second-order nonlinear optical properties that far surpassed those of the conventional materials has led to the synthesis and evaluation of a wide range of potentially useful solids materials showing high optical non linearity. Research has shown that the second-order nonlinear optical properties of organic crystal materials are closely related to their molecular structures. Among many organic compounds the second harmonic generations of Benzylidene aniline derivates are noticeable materials for the excellent green light transmittance and good crystal stability. In the present work a comparative study of 4-chloro 4′-methyl benzylidene aniline and 4-bromo 4′-methyl benzylidene aniline nonlinear optical single crystals are reported. The details of the experiment and the results will be discussed in detail.

Keywords: Benzylidene aniline, Organic Crystal, Second Harmonic Generation, Stability.

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DOI: https://dx.doi.org/10.5281/zenodo.1169107

Effect of Perchloric acid on Growth and Physical characteristics of Potassium Dihydrogen Phosphate Nonlinear Optical Crystals

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Abstract

Potassium dihydrogen phosphate is well known nonlinear optical material for various optoelectronics applications. Potassium dihydrogen phosphate continues to be interesting materials both academically and industrially. The overwhelming success of molecular engineering in controlling nonlinear optical properties in last decade has prompted better initiative in crystal engineering. In the present study single crystals of pure and perchloric acid doped potassium dihydrogen phosphate in different ratios has been synthesized by slow evaporation solution growth technique. The synthesized products are characterized by X-ray diffraction, Fourier Transform Infrared, UV-VIS-NIR, thermal analysis and micro hardness studies. The crystalline property and cell parameters of the grown crystals are studied by X-ray diffraction analysis. The shifting in frequency assignment of different functional group of Potassium dihydrogen phosphate due to addition of perchloric acid is analyzed by Fourier Transform Infrared spectroscopy. Transmission of light radiation from the grown material is identified from UV-VIS-NIR studies. Melting point of the grown crystal is obtained using melting point apparatus. Micro hardness test carried out at room temperature revealed that the grown materials belong to soft category.

Keywords : Crystal from solution, Characterization, X-ray diffraction, Micro hardness.

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DOI: https://dx.doi.org/

Mechanical, Dielectric, Linear and Nonlinear Optical Characterization of Pure and Lanthanum Doped Zinc L-Alanine Tartrate Single Crystals

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Abstract

Single crystals of pure and Lanthanum doped Zinc L-Alanine Tartrate were grown by slow evaporation solution growth technique. The cell parameters were determined using single crystal X-ray diffraction method. To improve the physical properties of the Zinc L-Alanine Tartrate crystal, Lanthanum dopant was added by 2 mol%. ICP studies confirm the presence of Lanthanum in the grown Zinc L-Alanine Tartrate crystal. Transparency range of the crystal was determined using UV-VIS-NIR spectrophotometer. The functional groups of pure and doped Zinc L-Alanine Tartrate crystals were analyzed by FT-IR spectroscopy. Using Vickers micro hardness tester, mechanical strength of the material was calculated. Dielectric studies of pure and doped Zinc L-Alanine Tartrate single crystals were carried out. NLO property of the grown material is confirmed by Kurtz Perry powder technique. The doped Zinc L-Alanine Tartrate crystal is found to have efficiency higher than that of pure Zinc L-Alanine Tartrate crystal. Most of organic NLO materials have poor mechanical and thermal properties, resulting in the damage of crystal during processing. To avoid this drawback, a new type of NLO material has been grown from organic-inorganic complexes. L-Alanine crystals have increased attention for photo induced nonlinear optical effects and dispersion of the linear and nonlinear optical susceptibilities. In the present work, a systematic study has been carried out on the growth of pure and Lanthanum doped zinc L-Alanine Tartrate crystals.

Keywords: **Nonlinear Optics, Amino acid, Organic Material.**

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DOI: https://dx.doi.org/10.5281/zenodo.1169112

Defects in nanoporous Au: insights from variable energy positron Doppler broadening studies

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Abstract

The analysis of low energy positron beam experiments in terms of positron diffusion and positronium fraction, $f_{3\gamma/2\gamma}$ provides an opportunity to obtain information aboutpositron annihilation behaviour and depth-wise defect distribution in nanoporous solids such as nanoporous Au (1).Herein, we have applied the positron beam with energy$E$, in the range of 0.2-21 keV to study the positron diffusion behaviorinnanoporous gold,having two distinct states,positively charged as-dealloyed and electrochemicallyreduced.It has been revealed from the analysis of the positron annihilationγ-ray spectra that the positronium fraction, $f_{3\gamma/2\gamma}$ with E in as-dealloyed nanoporous Au and bulk Au is found to be the same, whereas that obtained in reduced nanoporous Au is significantly increased(c.f. Fig. 1c).The increased positronium fraction,$f_{3\gamma/2\gamma}$ in reduced nanoporous Au is due to the absence of repulsive potential felt by thediffusing positrons at the surface of Au ligaments.

Keywords:electrochemical dealloying; nanoporous gold; slow positron; positronium fraction

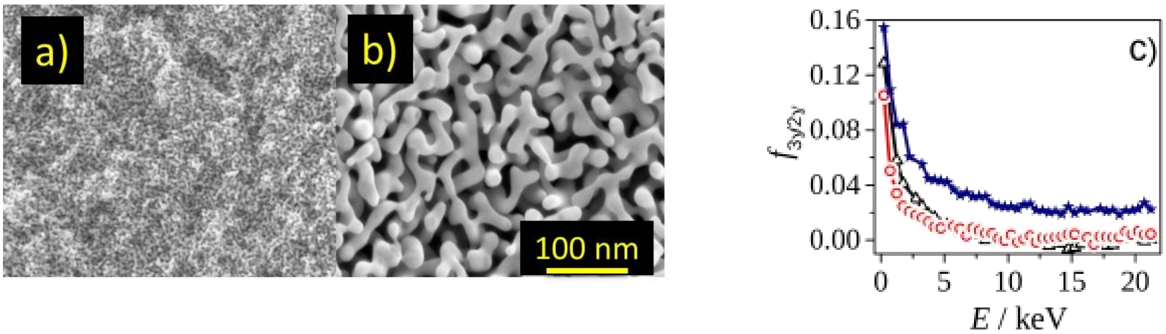

Fig. 1:a, b)Typical scanning electron microscopy images of positively charged as-dealloyed and electrochemically reduced nanoporous gold respectively. c)Positronium fraction$f_{3\gamma/2\gamma}$*vs.* positron incident beam energy E,foras- dealloyed (○), electrochemically reduced (*) nanoporous Au and defect freebulk Au (△).

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DOI: https://dx.doi.org/10.5281/zenodo.1169115

Synthesis of $CdWO_4$ nanoparticles by co-precipitation method

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Abstract:

Transition metal tungstates of $M^{2+}WO_4$ type (M^{2+} = Co, Cu, Cd, Mn, Pb and Zn) are ternary oxide semiconductors that are attracting considerable attention because they exhibit interesting technological properties such as ferroelasticity, ionic conductivity, and photoluminescence. Cadmium tungstate ($CdWO_4$) with a monoclinic wolframite structure belongs to the important family of metal tungstates. The present work report the synthesis of $CdWO_4$ nanoparticles using Co-precipitation method. The chemicals used for the synthesis of $CdWO_4$ nanoparticles were sodium tungstate and cadmium acetate. The synthesised white powder was calcined at 500°C for 2 hrs. The synthesized sample was investigated by XRD, FT-IR, UV-Vis, PL and SEM-EDX to identify its various properties. The XRD analysis confirmed the formation of monoclinic structure of $CdWO_4$. The band gap value of $CdWO_4$ was found to be 3.07 eV using Tauc's plot. The EDX study proved the purity of synthesized product.

Keywords: Metal tungstate, $CdWO_4$, monoclinic wolframite structure

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DOI: https://dx.doi.org/10.5281/zenodo.1169117

Quasicrystal: A remarkable catalyst for hydrogen production and hydrogen storage

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Abstract

The energy demand using more efficient or clean alternative energy sources will not only save the planet from harmful effects caused by pollution but could also reduce disparity and create a more peaceful world. The nanopartials, nanotubes and 2D materials have been proposed as catalyst for energy generation and storage because of their extraordinary properties and ease of production. In order to achieve this information, we have attempted to create a simple model catalyst of two dimensional layer of nano particles on quasicrystalline surfaces by leaching well defined surfaces of single grain quasicrystals. As the first step of these studies, we present here the effect of leaching treatments on surface morphology and chemical composition of different Al-based quasicrystals studied by scanning electron microscopy (SEM), energy dispersive x-ray (EDX) analysis and x-ray photoelectron spectroscopy (XPS). The high symmetry surfaces of single grain icosahedral (i)-Al-Cu-Fe and decagonal (d-) Al-Ni-Co, (d)Al-Cu-Co quasicrystals and a polygrain (i)-Al-Pd-Re, (i)-Al-Cu-Fe, (i)-Al-Pd-Mn quasicrystal with random surface orientation were leached with NaOH solution at varying times and the resulting surfaces were characterized by scanning electron microscopy, energy dispersive x-ray analysis and x-ray photoelectron spectroscopy. The leaching treatments preferentially remove Al producing nano-particles of the transition metals and their oxides. The leached fivefold surface of i-Al-Cu-Fe exhibits micron sized dodecahedral cavities on which the nano-particles are precipitated. However, no specific microstructure has been observed on the tenfold surface of d-Al-Ni-Co and the polygrain i-Al-Pd-Re. Quasicrystalline surface can be regained after polishing the leached layer, indicating that leaching occurs only in a limited depth from the surface. The use of such 2-D nanomaterials for hydrogen production will be discuses and presented in detail, explaining how their remarkable properties can enhance the efficiency hydrogen production and storage. The 2 hour leached as grown and mechanically activated Al-Cu-Fe layer materials was subjected for catalyst application in hydrogen storage materials for MgH2. The catalytic effect of leached alloy on the de/rehydrogenenation characteristics has been studied. The hydrogenation behaviour including absorption kinetics will be discussed and presented in detail.

Keywords: 2-D nano-materials; quasicrystal; hydrogen production; hydrogen storage.

DOI: https://dx.doi.org/10.5281/zenodo.1167607

Investigations on Intercalation Mechanism of Potassium Ion in Layered $Na_2Mn_3O_7$

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Abstract:

Li-ion batteries (LIBs) established as ubiquitous power source, especially in last three decades. LIBs may suffers from rarity and uneven distribution of resources, which limits their large scale applications. As alternative, potassium ion battery seize the attention of the scientific community due to high negative potential (-2.93V vs SHE) of the cathode materials next to Li-ion and almost having equal abundance like the Na-ion. Very recently, interesting result based on K-ion intercalating behavior of P2-type Na_xCoO_2 was demonstrated by sada et al., (1). However, research on layered oxide electrodes for K-ion battery is in an embryonic phase (2). In our work, we have investigated K-ion intercalation performance of layered $Na_2Mn_3O_7$ for the first time. The $Na_2Mn_3O_7$ was synthesized by conventional solid-state technique using $NaNO_3$ and $MnCO_3$ as precursors salts (3). Formation of triclinic symmetry P-1 with $[Mn_3O_7]_{2-\infty}$ layers fashioned with edge sharing octahedral of MnO_6 was confirmed from X-ray Diffraction and refined the structure using GSAS software. The systematic electrochemical studies were carried out by assembling a K-ion half-cell with K-metal as anode and $Na_2Mn_3O_7$ as active material in 0.8 M KPF_6 non-aqueous electrolyte. The fully K-ion intercalated structure $Na_{2-x}K_xMn_2O_7$ (x=2) was delivered a reversible capacity of ~108 mA h g^{-1} and good rate performance with columbic efficiency of ~95 %. The Ex-situ XRD measurements confirmed the phase transition and K-ion (de)intercalation. The detailed intercalation mechanism in lamellar type of $Na_2Mn_3O_7$ will be discussed.

Keywords: $Na_2Mn_3O_7$, Potassium-ion battery, Capacity, Cathode, layered structure.

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DOI: https://dx.doi.org/10.5281/zenodo.1169121

Investigation on Structural, Optical and Room Temperature Dilute Magnetism in Nanoscale Co and Fe co-doped SnO_2

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Abstract:

SnO_2 nanoparticles exhibiting room temperature ferromagnetism (RTFM) have been prepared by citrate gel combustion method. The saturation magnetization (M_s) of the nanoparticles experiences an increasing trend with an increase in Co and Fe dopant concentration. The annealing temperature also affects the oxygen vacancies which is also responsible for the origin of the Room Temperature Ferromagnetism. The structural, surface morphological, optical and magnetic studies were carried out using XRD, FESEM, UV–vis-NIR spectroscopy, photoluminescence and VSM. The tetragonal rutile structure of SnO_2 was confirmed using XRD data and it was found that this structure was not affected by Co and Co:Fe co-doping. It was observed that the magnetization increased with Co doping whereas decreased marginally after Co:Fe co-doping. The bound magnetic polarons resulted from the oxygen vacancies play a key role in the observed room temperature ferromagnetism.

Keywords: Diluted Magnetic Semiconductors, Room Temperature Ferromagnetism, BMP

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DOI: https://dx.doi.org/10.5281/zenodo.1169123

Structural, electrical and optical properties of Ba, Ni modified $KNbO_3$semiconducting ferro electric ceramics

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Abstract

Ferroelectric semiconducting ceramics with band gap (E_g)< 2 eV will be very useful for thephotovoltaic and photocatalytic application. Unfortunately all the current ferroelectric oxides have wide band gaps (E_g>2.7 eV for $BiFeO_3$, E_g>3.5 eV for PZT) [1,2] and can utilize only about 8%–20% of the solar spectrum and efficiency is very small. Recently, Grinberg et al. [3,4] invented a complex ceramic solid solution of $KNbO_3$-$BaNiNbO_3$ (KN-BNNO) which is ferroelectric and has a band gap < 2 eV. However, the problems associated with the development of the $KNbO_3$-based materials lies on its complex densification behavior and alkali evaporation leading to poor density. There are no literatures available for the preparation of dense KN-BNNO ceramics and it's electrical characterization.The presentpaper reports the effect of Ni doping and Ba, Ni co-substitution in $KNbO_3$ on phase evolution, electrical, optical properties and photocatalytic behavior.The temperature dependence dielectric permittivity of modified $KNbO_3$ ceramics indicates that the doping level significantly modifies the phase transition temperature. Impedance spectroscopy is used to understand the electrical conduction behavior with doping and temperature. UV-Vis absorption spectroscopyindicates thatNi-doped and Ba-Ni co-doped $KNbO_3$ have significant absorption in the visible range. Photocatalytic activity evaluation displays an enhanced visible light photocatalytic activity of Ba-Ni co-doped $KNbO_3$ in degrading rhodamine B in comparison with $KNbO_3$.

Keywords: $KNbO_3$; Doping; Electrical properties;

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DOI: https://dx.doi.org/10.5281/zenodo.1169129

Effect of High Pressure on structural and vibrational stability of Co and Li doped ZnO ($Zn_{0.90}Co_{0.05}Li_{0.05}O$) nanoparticles

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In this paper, we report the pressure effect on synchrotron XRD and Raman measurements of $Zn_{0.90}Co_{0.05}Li_{0.05}O$ nanoparticles to understand its structural and vibrational stabilities under high pressure (HP) at room temperature. The selected samples were prepared using a co-precipitation method, and the quality of nanocrystalline phases were confirmed by a Bruker D2 phaser XRD diffractometer, Surface morphology of the prepared nanoparticles were carried out using a SEM [1]. The HP XRD was performed up to 28 GPa, and PV phase diagram was obtained with Third order BM EoS. The structural phase transition from hexagonal Wurtzite to cubic rocksalt structure is observed with the critical pressure range of 11.12 to 16.64 GPa, and the bulk moduli are 178 and 255 GPa^{-1} for these phases respectively. In this range, a mixed phase of both structures was observed. This same phenomenon has been observed in high pressure Raman measurements. Comparing with the lit., the critical phase transition pressure of ZnO (9 GPa) [2] is enhanced to (11.12 GPa) by Li and Co doping. So, the substitution of these elements at the Zn site tend to occupy the interstitial sites rather than substitution sites, and acted as donors instead. Hence, the doping elements lead to *p*-type conductivity with an increase in the Zn-O bond distance. But, HP compresses the crystallite size, which leads to increasing the lattice strain and reducing the band gap of this semiconductor material. As a result of lattice strain hindrance up on compression, the larger ions rather than the smaller ions try to counteract the high pressure, due to ionic force repulsion within the lattice [3]. This study provides an efficient way to modify these types of semiconductor materials for technological applications.

Keywords: High Pressure, Synchrotron XRD, Raman modes, Structural Transition

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DOI: https://dx.doi.org/10.5281/zenodo.1169131

Silicon Carbide(SiC) Thin Film Deposited On Silicon- An Interesting NIR Emission

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Abstract:

Research on crystalline silicon carbide (SiC) thin film exhibits strong visible and NIR emission due to its wide band gap[1].Polymer derived SiC thin film has been of great interest due to its high thermal stability and good mechanical properties. This paper deals with deposition of SiC thin film on Silicon (Si) wafer using boron doped Liquid Polycarbosilane (PCS) by Modified Chemical Vapour Deposition (MOCVD).

The film was characterised by GA-XRD and X- ray photoelectron spectroscopy. The GA-XRD plot indicates formation of β-3C SiC Nano crystals. The binding energy diagrams obtained from XPS ascertain the presence of boron [2] and amorphous carbon into the SiC matrix.

Finally, The Photoluminescence spectra (PL) shows a unique NIR emission from 750 nm to 900 nm on excitation of 532 nm laser. This indicates that the boron doped SiC thin film on Si can be a promising material for the fabrication of different optoelectronic devices.

Keywords: Silicon Carbide; Nano crystal; Thin Film

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DOI: https://dx.doi.org/10.5281/zenodo.1169135

Molecular dynamics simulations of nanoindentation to evaluate the mechanical properties of various metallic alloy nanoparticles

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Abstract

We present here the procedure of molecular dynamics (MD) simulations of nanoindentation of various metallic alloy nanoparticles viz. copper-silver alloy and copper-nickel alloy with different alloy compositions. The crystals, pre-equilibrated at 298 K are subjected to indentation by spherical shape rigid indenter of specified diameter. For each case we have performed molecular dynamics simulation of a full indentation cycle which includes loading and unloading stages and based on the load-displacement curves we have calculated hardness and Young's modulus of the materials. The Embedded Atom Method (EAM) potential, which is proved to be reliable for metallic systems, has been used here for the interatomic interactions, both during nanoindentation and the prior thermal equilibration stage. During the process of nanoindentation, the resultant load (P) in the nanoparticle has been calculated by summing up the fz component of force of each atom at each time step. The corresponding displacement (h) of the indenter has been calculated taking the centre of mass of the indenter once it touches the nanoparticle's top surface, as the reference.The results indicate the role of surface effect and composition effect in influencing and young’s modulus of the alloy nanoparticle. The present work played an evident role for the estimation of mechanical properties of nanoparticles by MD simulations of the nanoindentation process.

Keywords: **Molecular dynamics; Nanoindentation; Mechanical properties; Young's modulus; Alloy nanoparticles**

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Acknowledgment: The financial support of Centre of Excellence under TEQIP-II is thankfully acknowledge

DOI: https://dx.doi.org/

Impact of sintering temperature variation on the structural and electrical properties of praseodymium modified $Ba_{0.85}Ca_{0.15}Zr_{0.1}Ti_{0.90}O_3$ ceramics

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Abstract

Rare-earth ions like praseodymium (Pr) substitution has been shown to enhance the electrical properties of lead free piezoelectrics [1 – 4]. The effect of sintering temperature variation (1350 – 1450 °C) on the structural, ferroelectric and dielectric properties of0.04 wt% Pr_6O_{11}-doped $Ba_{0.85}Ca_{0.15}Ti_{0.9}Zr_{0.1}O_3$ (BCZT) ceramics has been studied systematically. The results demonstrated that structural and electrical properties of Pr modified BCZT samples are strongly sintering temperature dependent. XRD results confirmed co-existing tetragonal and orthorhombic phasesat all sintering temperatures with maximum tetragonality at 1400 °C. Further, the average Ti – O bond length decreases with increasing sintering temperatures.Similar observations were made from the Raman spectra. The highest ferroelectric ($2P_r$ ~ 21.6 μC/cm^2) and dielectric (ε_m ~ 8805,tanδ ~ 0.032) properties were observed for Pr doped BCZT compound sintered at 1400 °C.The electrical properties are explained on the basis of crystallite size, density, tetragonality and bond length of these ceramics. It is concluded from the present study that optimal properties of 0.04 wt% Pr_6O_{11}-doped BCZT can be achieved at 1400 °C sintering temperature.

Keywords: Lead free ceramics; Ferroelectric properties; Dielectrics properties

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DOI: https://dx.doi.org/10.5281/zenodo.1169144

Preparation and characterization of magnetic nanoparticle encased fluorapatite nanostructure for biomedical applications

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Surface modification of magnetic nanoparticles (MNP) is important in biomedical applications for improving their effective biodistribuion, hydrophilicity, colloidal stability, biocompatibility and conjugation of bioactive functional groups. There are numerous organic and inorganic materials used for coating the surface of MNP. The harsh *in vivo* conditions may lead to the disappearance of the organic surface coatings and also the utilization of organic solvent as reagents for generating the organic coatings is a concern from the toxicity point of view. Hence surface modification using inorganic materials may be more effective.

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Fluorapatite [FAP, $Ca_{10}(PO_4)_6F_2$]can be a most promising inorganic material for the surface modification of MNP. Surface modification of iron oxide (Fe_3O_4) and zinc ferrite ($ZnFe_2O_4$) nanoparticles with biocompatible FAP coating achieved by hydrothermal method will be discussed. TEM images revealedMNP encased rod shaped FAP nanoparticles. FAP coated MNP enhanced the cell viability and colloidal stability when compared to MNP. Magnetic measurements of the prepared samples exhibit superparamagnetic nature at room temperature. These results demonstrate that FAP coated MNP could be a suitable candidate for drug delivery, hyperthermia and MRI contrast agent.

Keywords: Magnetic nanoparticles, Fluorapatite, Superparamagnetic

DOI: https://dx.doi.org/10.5281/zenodo.1169197

X-ray diffraction and Optical studies of ZrO_2 Thin films prepared by Spray Pyrolysis Method

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Abstract

Thin film of zirconium oxide on glass substrate was prepared by spray pyrolysis method. Film thickness is determined by viewing cross section image from Scanning Electron Microscope. It is found to be 1.051 micron for the film prepared at 250°C. X-ray diffraction pattern indicate the material is of crystalline in nature with preferential orientation along (1 1 1) plane having grain size of 18 nm. Optical transmittance is studied using spectrophotometer in the wavelength range 380 - 800 nm. Optical transmittance curve shows a linear increase towards higher wavelength region and indicating crystalline nature of the film. Also optical transmittance has 85% in the higher wavelength region. Energy band gap of the film is obtained by plotting graph hν Vs $(\alpha h\nu)^2$ and is found to be 2.57eV indicating semiconductor nature. The results thus obtained will be discussed in detail.

Keywords: Spray Pyrolysis, Energy band gap, Thin film, X-ray diffraction.

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DOI: https://dx.doi.org/10.5281/zenodo.1169201

Facile synthesis of Room temperature LPG sensor based on Nano structured composite of Graphene oxide and SnO_2 anchored with PANI.

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Abstract

In this present work, a LPG sensor based on ternary nano- hybrid of (PANI–SnO2/GO) has been synthesized via wet chemical route. The crystal structure, Morphologies and composite are examined by various characterizations techniques such as UV-Visible spectroscopy, X-Ray diffraction, Fourier-transform infrared spectroscopy, and Scanning electron microscope. The gas sensing behavior of the nano composite were analyzed by exposing different ppm at room temperature. The composite shows good sensitivity towards the flow of LPG and it has improved response and recovery time. This composite have selective towards LPG against oxygen and hydrogen. The addition of conducting polymer PANI in the ternary structures modulates the electron transfer between the composite towards the gas molecules at room temperature. This synthesized composite has promising advantages in the field of gas sensor by means of reduced operating temperature ease of fabrication and low cost.

Keywords : Ternary hybrid, Gas sensor, Nano structured Composites, LPG Sensor

DOI: https://dx.doi.org/10.5281/zenodo.1167614

Effect of NaCl on Structural, Spectroscopic and Optical properties of Methyl Orange Doped Urea L-Malic Acid Crystal

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Abstract

Non linear optical single crystals of NaCl and methyl orange doped urea L-malic acid crystals were grown by slow evaporation technique. Good quality single crystals of dimension 10×9×2 mm^3 and 10×9×2 mm^3 are harvested in 20 and 30 days respectively. Influence of dopants in urea L-malic acid was studied. The grown crystals are characterized by single crystal X-ray diffraction. The study reveals that the crystal belongs to monoclinic system with $P2_1$ space group. The structures of the compounds are further confirmed by Fourier Transform Infrared spectra. The effect of optical properties on doping and the transparency of the grown crystals are analyzed by UV-Visible spectra. The micro hardness study shows that the Vickers hardness number of the crystal decreases with increase in applied load. The nonlinear optical test confirms the second harmonic signal generation in the sample.

Keywords: Single Crystal, Slow Evaporation, Monoclinic, Microhardness.

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DOI: https://dx.doi.org/10.5281/zenodo.1169203

Optimization of microwave irradiated synthesis parameters of eggshell derived hydroxyapatite at lab scale

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Abstract

Hydroxyapatite (HAp) is a calcium phosphate bioceramic material which forms major inorganic component of human hard tissues (bones and teeth). It is widely used as bone substitutematerial in orthopedic and dental applications. Also it has an excellent biocompatibility, osteoinductivity and ability to promote osteoblast functions. There are several reports on the synthesis of HAp from biogenic biowaste minerals such as marine shells, snail shells, mussel shells and eggshellsusing direct and indirect conversion methods. The microwave synthesis of ceramics has several advantages including shorter synthesis time, fast reaction, easy reproducibility, narrow particle size distribution, etc. Phase pure HAp powder was synthesized by lab scale microwave irradiation method using eggshell as the calcium precursor. The optimizationof synthesis parameters such as pH, microwave power, volume and EDTA concentrationswill be discussed.

Keywords: Hydroxyapatite, Eggshell and Microwave irradiation

DOI: https://dx.doi.org/10.5281/zenodo.1169205

Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials

Structural and microwave absorption properties of chemical vapor deposited MWCNTs in the 8-12 GHz region

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Abstract:

In this Era, effort has been made to develop different forms of carbon using natural carbon source camphor and study their microwave absorption properties in the 8-12 GHz region. Peaks observed at 2θ = 25.6° and 43.5° are assigned to the graphitic phase of carbon with (002) and (100) diffraction planes. The SEM study shows the formation of MWCNTs at an optimum temperature of 900°C. After 900°C temperature, there is sudden increase in the diameter distribution of MWCNTs. TEM study depicts that at 900°C, the diameter of MWCNTs is minimum and they are contaminated with very few metal catalyst particles. In the Raman spectrum G-band centered at 1594 cm^{-1} indicates the presence of a hexagonal graphitic structure of MWCNTs. The microwave properties have been carried out in the 8-12 GHz frequency region. MWCNTs grown at 900°C shows the high reflection loss (RL) value of -33.56 dB (>99.9% power absorption) at 11.8 GHz however, they exhibit maximum SE value of -65.22 dB at 8 GHz and -46.27 dB at 10.19 GHz. Also, MWCNTs shows maximum microwave attenuation up to 65.84 dB in the 8-12 GHz frequency range.

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DOI: https://dx.doi.org/10.5281/zenodo.1169207

Transport of Indomethacin from carrageenan-gelatin nanogel

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This paper describes a single emulsion-solvent evaporation method to prepare biocompatible nanogel carriers by utilizing different concentrations of carrageenan and gelatin. The gels were characterized based on average particle size, zeta potential, SEM and release patterns. It was found that average particle size was in the range of 2000- 4000 nm after drug entrapment. An effort has been made to investigate release kinetics of Indomethacin (model drug) to study the transport from the nanogel carrier matrices. The entrapment efficiency was found to be nearly 40%. UV-visible spectrophotometric method was used for estimation of indomethacin content in the formulation. The prepared formulation exhibited 90% cumulative drug release for up to 24 hours.. The cytotoxicity study was performed for carrageenan & gelatin combinations on MCF7 breast cancer cell lines using MTT assay and the results suggest that the nanogel did not impart any significant level of toxicity. Therefore, the nanogel carriers could be exploited to entrap other therapeutic agents as well as growth factors. Overall, all the results prove the gels could be tuned to be a good candidate for biomedical applications.

Keywords: biopolymer, carrageenan, gelatin, nanogel,drug release

DOI: https://dx.doi.org/10.5281/zenodo.1169210

Magnetic and transport properties of Gd and Cr co-substituted $SrRuO_3$

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Abstract

We explore the crystal structure, electrical resistivity and magnetic behavior of the compositional series $(SrRuO_3)_{1-x}$ $(GdCrO_3)_x$ (where, $0 \leq x \leq 1$) with the evolution of x, which resides between orthorhombic ferromagnetic (FM) metal $SrRuO_3$ (T_C = 160 K) and orthorhombic antiferromagnetic (AFM) insulator $GdCrO_3$ (T_N = 170 K). Crystal structure analysis reveals that complete solid solution exists only up to $x = 0.1$, and above which chemical phase separation of two/three phases occur. Electrical resistivity measurements affirm the temperature driven metal to insulator (*M-I*) transition for $x = 0.05$ and 0.1 samples. Low temperature insulating state in these samples are interpreted by electron-electron interaction of weak disordered systems. Precise analysis of temperature dependent resistivity for $x \geq 0.2$ samples (which have insulating ground state) dictate that transport phenomenon is mainly associated with the Arrhenius-type charge conduction, Mott's variable range hopping, short-range and long-range Coulomb interaction mediated hopping processes due to high degree of randomness. A strong hybridization between 4*d*(Ru) and 3*d*(Cr) orbital enhances the value of T_C up to $x = 0.1$. The effective magnetic moment (μ_{eff}) continuously increases with the incorporation of higher moment elements (Gd and Cr).

Keywords : Band and Itinerant models, Localization effects, Magneto-transport

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DOI: https://dx.doi.org/10.5281/zenodo.1169212

Development of superhydrophobic magnetic nanocellulose sponge for oil/water separation

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ABSTRACT

Tackling of severe environmental issues emerging from oil spill accidents and industrial oily waste water is a challenging task (1). Recently, sponge like 3D materials with superhydrophobic and superoleophilic properties have attracted considerable interest in the field of oil water separation owing to their excellent sorption capacity and high selectivity of oil (2-4). Herein, we have successfully fabricated Superhydrophobic and superoleophilic cellulose sponge from paper waste via freeze drying followed by silanization and achieved water contact angle >150^o and oil contact angle nearly 0^o. Fe_3O_4 nanoparticles were integrated on the surface of the cellulose sponge which facilitated collection of the sponge after oil separation. Morphological analysis was performed using Scanning Electron Microscopy. Oil absorption capacities, magnetic and mechanical properties of the sponge have been evaluated. The superhydrophobic magnetic nanocellulose sponge could separate oil/water mixture with high separation efficiency and good reusability.

Keywords: Superhydrophobicity, cellulose sponge, silanization, oil/water separation

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DOI: https://dx.doi.org/10.5281/zenodo.1169217

Microave dielectric relaxation spectroscopy studies on polar –polar binary liquid mixtures of triethylene glycol with ethyl butyrate.

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Abstract

The complex dielectric spectra of triethylene glycol with ethyl butyrate and their binary mixtures were measured in the frequency range of 10 MHz to 50 GHz at various temperatures using Time Domain Reflectometric (TDR) technique. The dielectric parameters (static permittivity and relaxation time) were extracted from the complex permittivity spectra by using least square fit method. Debye relaxation model is suitable for extracting the dielectric parameters. The derived static permittivity (ε) and relaxation time (τ) values were used to calculate various dielectric parameters like excess dielectric constant, effective Kirkwood correlation factor, excess inverse relaxation time and thermodynamic parameters. Excess dielectric parameters were fitted with the Redlich–Kister type polynomial equation. The result of dielectric relaxation studies confirms the formation of a heterogeneous complex structure by association of unlike molecules and may also intra molecular interaction possible between similar molecules. Molecular rotation and dipole reorientation motions in these complex systems are discussed in terms of the molar activation entropy and enthalpy. Additionally, the hydrogen bond interaction between solute and solvent were confirmed by FT–IR spectral analysis.

Keywords: Complex permittivity, dielectric constant, molecular interaction, Effective dipole, enthalphy.

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DOI: https://dx.doi.org/10.5281/zenodo.1169222

Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials

Comparative Study of Lithium ion Batteries for Electrical Vehicles system

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Abstract

Current lithium ion battery technology is ready to revolutionize hybrid vehicles. Lithium iron phosphate batteries have twice the specific energy than that of nickel metal hydride batteries used in current hybrid vehicles. The batteries are also capable of enormous amounts of power, up to 3.3 kW/kg. This makes it possible for higher performance hybrids that are more appealing to the average consumer. The study presents a techno-economic comparison of the most commonly used battery technologies such as lead iron batteries and lithium cobalt batteries. Lead is a very heavy metal and therefore the research was done from many years to make better battery that is lighter in weight as well as it has improved power density. Then lithium became the logical choice to replace lead as it is the lightest metal available in the world. Lithium is not only light in weight but also highly reactive and for this reason pure lithium is never found in nature. In today's world Lithium Ion batteries are used in almost all gadgets including laptop, cell phone, camera, iPod and many more devices and hence they are very popular these days. They are one of the most energetic batteries available today which make them so popular. Our major concentration is on Lithium Iron Phosphate batteries and Lithium Cobalt batteries.

Keywords: Lithium ion Battery, Lithium Cobalt Battery, Power Characteristics.

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DOI: https://dx.doi.org/10.5281/zenodo.1169225

Synthesis, Growth and Characterization of Semi Organic Nonlinear Optical Single Crystals of Sodium Dihydrogen Orthophosphate Hippurate

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Abstract

Semi Organic nonlinear optical crystal of Sodium Dihydrogen Orthophosphate Hippurate (SDPH) was synthesized and the crystals were grown by slow evaporation solution growth technique at room temperature using ethanol as solvent. The grown crystals were characterized by Single crystal XRD, Powder XRD, FTIR, UV- VIS - NIR and fluorescence spectral analyses. The crystal structure and lattice parameters were determined by single crystal XRD. The powder X-ray diffraction pattern shows a high degree of crystallinity of the grown crystals. The FTIR spectrum was recorded in the region 1450 - 4000 cm^{-1} to identify the presence of functional groups. UV - VIS - NIR spectral analysis shows 98% transmission in the entire visible region. Fluorescence spectrum recorded shows a peak at 528 nm. Mechanical properties of the grown crystals were studied using Vicker's micro hardness tester. The SHG efficiency of SDPH was measured by the Kurtz powder technique and the grain size was confirmed by SEM.

Keywords: Organic Compounds, Fluorescence, X – ray diffraction, SHG Efficiency.

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DOI: https://dx.doi.org/10.5281/zenodo.1169232

Study of Lead Acid Batteries in Photovoltaic Systems

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Abstract

Battery is a crucial component in a photovoltaic system. It provides energy for the loads during night or non sunny days. It can be considered as a stabilizer. Most of the batteries used in photovoltaic systems nowadays are lead acid batteries. The study of a photovoltaic system necessitates in a first time equivalent models of the main components such as photovoltaic generator model, storage element. The knowledge of their electrical characteristics remains a key factor in the simulation analysis. The battery behavior has been largely described in the literature by many authors. Most of the models require the knowledge of appropriate parameters. Batteries remain a complicated element, since they are the only dynamic element in a photovoltaic system. In fact many events can occur such as charge and discharge. Many parameters vary during the processes of voltage, current, density, temperature and resistivity. The CIEMAT model is general and normalized with battery capacity, it necessitate few input parameters. It takes into account the discharge, the charge and the overcharge processes and it can be applied for wide range of lead acid batteries used in photovoltaic systems. The CIEMAT model presents a good performance to represent dynamic and complex battery operation. This paper reviews the general lead acid batteries model and it agreement with experimental data obtained from tests with in photovoltaic systems.

Keywords: Photovoltaic System, Resistivity, Voltage, Electrical Characteristics.

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DOI: https://dx.doi.org/10.5281/zenodo.1169234

Reducing gas sensing property of polypyrrole/polyaniline conducting polymer blends synthesized by interfacial polymerization

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Abstract

Polypyrrole/Polyaniline conducting polymer blends as room temperature operated hydrogen gas sensor were fabricated using simple inexpensive Interfacial Polymerization method. Synthesis of polypyrrole and polyaniline conducting polymers were achieved by the interfacial polymerization. Miscible and Immiscible conducting polymer blends were synthesized by one step and two step polymerization methods respectively (1, 2). The Glass Transition Temperature (T_g) of the conducting polymer blends were determined by Thermo gravimetric Analysis (TGA) and Differential Scanning Calorimeter (DSC). Surface morphological studies were characterized by the Scanning Electron Microscope (SEM) and Transmission Electron Microscope (TEM). Structural studies were done by the X-ray Diffraction (XRD), Fourier Transform Infrared Spectroscope (FTIR) and UV-visible absorption Spectroscope. The polymer blends showed selectivity towards hydrogen among oxygen and Liquid Petroleum Gas (LPG). It also revealed improved sensor characteristics such as sensitivity, response time and recovery time. The fabricated electrodes are highly stable for the period of 50 days.

Key Words: Polypyrrole/Polyaniline Blends, Interfacial Polymerization, Hydrogen Gas, Sensitivity

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DOI: https://dx.doi.org/10.5281/zenodo.1167620

Morphological and electrical studies of Graphite nanostructures and its biological applications

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Man has created several artificial forms of carbon some of these are: synthetic graphite and synthetic diamonds, adsorbent carbon and graphitic fibers, glassy carbons, diamond-like carbon, etc. These are used nowadays for application in various forms like electrodes and electrical contacts, lubricants, shoe polish, gemstones, high performance tennis rackets, aircraft and spacecraft composites, heat sinks for ultrafast semiconductors, etc.[1]. By using hydrothermal method Graphite powder was prepared, the carbon source materials of graphite (flaky graphite), NaOH, Glucose we have synthesized fine nano rods of Graphite powder and its crystal size was calculated by using Scherer equation. Its value is equal to 72 nm and its predominant plane of (002) was confirmed by using the JCPDS file 75-1621 peaks were confirmed and well matched with the results. Band gap 5.38 eV value of the Graphite powder was analysed by UV-Vis Spectroscopy [2]. FTIR Spectrometer inferred that two main peaks located at about 963 -1474 cm^{-1} and 2369-3464 cm^{-1} which confirmed the formation of Graphite nanostructures. The FE-SEM and EDAX analysis demonstrate that the morphology changed from dense to fiber in hollow and hollow nano rods with increase the relative decreasing size of synthesized Graphite powder. Synthesized Graphite powder was used to study about the biological applications of antifungal activities of it [3].

Keywords; Graphite powder, Scherer equation, Glucose and FTIR

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DOI: https://dx.doi.org/10.5281/zenodo.1169238

Exploringtitanium based anode materials for M ionbatteries (M = Li/Na)

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Abstract

Lithium ion batteries (LiBs) have been at the major research focus of energy storage since the early90s. Lately, its ubiquitous overuse in portable electronics and rising cost has paved way for research on earth-abundant sodium ion batteries (SiBs), whereby finding new redox active materials have become imperative. A myriad of mid-range voltages can be accessed through the same Ti^{4+}/Ti^{3+} redox couple in differentTi based compounds. This is due to their diversity instructural framework andchemically dependent ionicity of the Ti-O bond. They offerample scope for use both in LiBs, as anodes and cathodes, in SiBs, as anodes and bipolar electrodes in $NaTi_xM_yO_2$ (M=Cr/Mn/Fe/Co/Ni/Ru) with the additional M redox activating in the positive electrode (1). The mid voltage regime helps safely prevent risk of platingand a low volume change ensures extreme rate capabilities. This is best seen in$Li_4Ti_5O_{12}$ defect spinel and $MLi_2Ti_6O_{14}$ (M=2Na, Sr, Pb) that reversibly store lithium in afast stable bi-phase flat plateauwithvery low polarization. Our group has taken a significant step toward by showing good reversiblelithium intercalation in $SrLi_2Ti_6O_{14}$and $Na_2Li_2Ti_6O_{14}$(2,3), synthesized in energy efficient, combustion and sonochemicalsynthesis requiringvery lowtemperature and time. Selecting anodes and cathodes with a wider voltage window maximizes the energy density. A way to do this is by reducing the voltage of anodes. However, due to the inactivity of graphite and a progressive capacity fade seen in hard carbon,increasing effort is directed towards findingnew suitable low voltage anode materials. In this regard, similar to $Na_2Ti_3O_7$ introduced in 2011 (0.3V, 200 mAh/g), our group has shown good reversible sodium intercalationin combustion synthesized $Na_2Ti_6O_{13}$(40 mAh/g, 0.83V), furtherextending it as proof of concept thin film batteries for the first time (4). All these along with more recentwork on $PbTi_3O_7$(175 mA/g, 0.5V) as SiB and$Na_2TiSi_4O_{11}$(60 mAh/g, 0.5V) as LiB shallbe discussed.

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DOI: https://dx.doi.org/10.5281/zenodo.1169242

Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials

Development of an *in situ* consolidated nanocrystalline $Cu_{88}Al_{11.5}Y_{0.5}$ alloy

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Nanocrystalline $Cu_{88}Al_{11.5}Y_{0.5}$ bulk alloy has been synthesized by in situ consolidation of mechanically alloyed powder blend followed by annealing of the consolidated compact at 200° C (or 0.35 T_m) for 30 min. Grain size determination and phase identification have been carried by X-ray line broadening analysis and transmission electron microscopy (TEM). Hardness measurement has demonstrated that the Hall-Petch effect is the dominant strengthening mechanism for both as-consolidated and annealed specimens. Strength improvement after short annealing time was attributed to the relaxations of non-equilibrium grain boundaries.

Keywords: Nanocrystalline copper alloys, Mechanical alloying, In situ consolidation, strengthening mechanism

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DOI: https://dx.doi.org/10.5281/zenodo.1170654

Molecular dynamic simulation studies of thermal diffusion of lithium and lithium based alloys

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Abstract

Lithium and Lithium based alloys are widely used in the industry as an important source of renewable energy, for example, battery electrolytes, electrodes and catalysts. Despite huge research activities in past several decades, a detailed kinematic study of Li-ion within the material and the structural stability of the material are still lacking in the literature. Here we present a detailed study of the thermal diffusion of Li and Li_2O using molecular dynamic simulations software LAMMPS (1,2). Velocity verlet scheme is used for the time advancement of the system. Temperature dependence of diffusion coefficients D(T) for Li and Li_2O were computed. Activation energies (E_a) for both the material were determined using the Arrhenius relation $D=D_oe^{-Ea/KT}$. The obtained results are consistent with previous experimental and numerical observations (2,3). Furthermore, we create vacancies at the Li sites and investigate the role of the concentration of vacancies on the thermal transport of the material.

Thermal diffusion, Molecular dynamic simulation, Activation energy, Defects

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DOI: https://dx.doi.org/10.5281/zenodo.1170660

Europium doped YBO_3 luminescent pigment for security ink application

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Abstract

Herein, we report an orange-red colour emitting $YBO_3:Eu^{3+}$ phosphor, synthesized by Sol gel technique, which can be simply scaled up in large quantity. This highly luminescent and optically active $YBO_3:Eu^{3+}$phosphor with average particle size in the range from 100 to 120 nm provides emission at 591 nm upon 245 nm excitation wavelength and also excitable in range of 280-480nm excitation wavelengths. The structural/microstructural and photoluminescence behaviour were characterized by scanning electron microscopy, transmission electron microscopy/high-resolution transmission electron microscopy and fluorescent spectroscopy, respectively. Further, this nanophosphor was used to design luminescent security ink with commercially available polyvinyl chloride gold medium for printing of highly uniform security codes as investigated by PL mapping instrument. Thus, this facile method to synthesize a low cost $YBO_3:Eu^{3+}$ phosphor based security ink offers a nonreplicable security codes for printing that can be easily printed but is difficult to duplicate.

DOI: https://dx.doi.org/10.5281/zenodo.1170665

Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials

Microwave Properties of Screen Printed Carbon Nanotubes Thick Film

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Abstract

Carbon nanotubes have been received more attention due to their excellent electrical properties and lightweight nature. For their use in the microwave frequency region, these MWCNTs are transformed into planar form. In the present study, the properties of MWCNTs thick film on alumina substrate has been reported for the first time by the screen printing method. The functionalization process of MWCNT with acid solution resulted into the reduction in agglomeration and surface modification of CNTs with carboxyalic groups. The thickness obtained for the present MWCNT thick film is around 10 μm. The MWCNT were thermally stable in nitrogen atmosphere up to 750 °C. The X-ray diffraction pattern of MWCNT thick film shows two characteristic graphitic peaks at 26.5° and 54.7° corresponding to (002) and (004) reflections. The real and imaginary microwave permittivity of MWCNT thick film from the straight resonator overlay method were 6.6 and 17.6 respectively

Keywords – Multiwalled carbon nanotubes, Screen printing, Thick film, Microwave permittivity

DOI: https://dx.doi.org/10.5281/zenodo.1170670

Effect of Mn dopingon conductivity and Photocatalyticbehaviourof $SmFeO_3$

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Abstract

Ferrites and orthoferriteshave attract researchinterest as an eco-friendly material to substitute toxic lead based perovskitesin various applications (1). The Mn doped $SmFeO_3$ (SFO) were prepared by facile sol-gel method which shows distorted type of structurein the space group Pbnm (2). The Ac conductivity has been measured which shows an increasing tendencywith the temperature,indicates the semiconducting behaviour of the material. Hence, a semiconductor to metallic transition at the temperature 723 Khas also been found.The visible light induced photocatalytictestswere performed by the degradation oforganic pollutantRh-B and the result reflects that the apparent rate constant (K) has been increased with higher amount ofMn concentration. Additionally, higher Mn doping causes decrease in band gap from 2.60 eV to 1.82 eV. The enhanced photocatalytic activity and conductivity of the material may happen due to Mn doping which enhance the active catalytic sites.

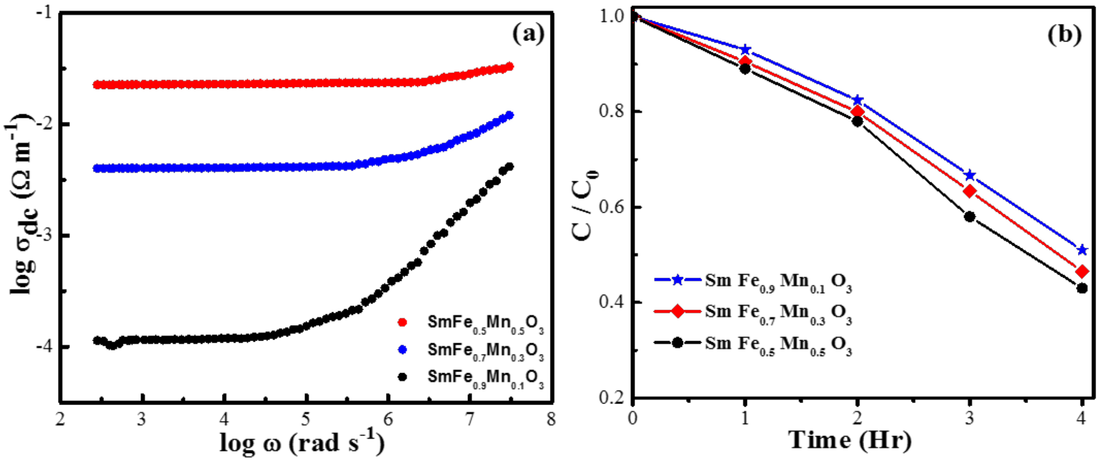

Fig : (a) The Ac conductivity at room temperature and (b)the Photocatalytic degradation of RhB as a function of the irradiation time under visible light for the as-prepared Mn-doped SFO samples.

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DOI: https://dx.doi.org/10.5281/zenodo.1170672

Thermal evaporation technique to prepare ZrO_2 doped TiO_2 thin film on Si Substrate

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Abstract

ZrO_2 and TiO_2 has much attention among the nanomaterials because of good compatibility of technological and biological activities. The two gram of Titanium isopropoxide ($[(Ti(OCH)(CH_3)_2]_4$) is mixed in 25 ml of water to prepare 1 M solution. Similarly 0.9 gm of ZrO_2 mixed with 15 ml of water to get 0.5 M solution. By using simple co-precipitation technique powder particle was prepared. This powdered particle was pelletized and then used it for target. It was allowed to raise the temperature up to 200^0C for 15 minutes. This pellet was evaporated by using this technique on Si substrate, it was characterised by using X-Ray diffractometers to study the analysis were performed to study the structural and optical properties. In XRD analysis some of the sharp peaks were observed and identified the presence of TiO_2 doped with ZrO_2 which is suggested the good crystallinity. This sample was used to measure the conductivity and resistivity of the prepared sample.

Keywords; Si substrate, Titanium isopropoxide, ZrO_2 and Thermal evaporation

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DOI: https://dx.doi.org/10.5281/zenodo.1170675

Plasma polymerized ultra-smooth polypyrrole thin film optical waveguide for integrated optics

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Abstract: An optical waveguide is the key solution in signal propagation as it avoids electromagnetic interference, provides high bandwidth and playing a key role in miniaturization as an immense part of integrated optics. In the current research work, ultra-smooth polypyrrole thin film has been deposited by non-thermal plasma polymerization method by varying input power. Polypyrrole thin film is characterized for structural, optical and mechanical properties. Surface morphology reveals its nanostructured grains which are arranged on a surface in a compact manner. The functional groups are confirmed by FT-IR analysis. π-π* transitions of electrons is confirmed from optical absorption peak at 340 nm. Optical waveguiding property of polypyrrole thin film is obtained by prism coupling method and found that, optical transmission loss is decreased with power applied and showed 6.28 dB/cm as minimum loss for the film deposited at applied power 12 watt. Adhesion of the polypyrrole thin film is increased, whereas absorption, refractive index, optical band gap, optical transmission loss and roughness of the film are found to decreases with power applied.

Keywords: Polypyrrole, Plasma polymerization, Optical waveguide

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DOI: https://dx.doi.org/10.5281/zenodo.1170679

Alkali Iron Phosphates as An Efficient Oxygen Reduction Electrocatalysts

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Abstract:

Water-Splitting systems are essential for clean energy production. The oxygen reduction reaction (ORR) is a key reaction involved in water splitting, which requires a catalyst. The current work explores the possible application of sodium and potassium iron phosphates ($AFePO_4$, A = Na, and K) as electrocatalysts for ORR activity. These earth-abundant iron phosphates were synthesized by solution combustion synthesis (SCS) technique using ascorbic acid both as fuel and reducing agent for Fe. The crystal structure was analyzed by Rietveld refinement. The formation of carbon coating was identified by thermogravimetric analysis and Raman spectroscopy. Electrocatalytic properties of $AFePO_4$ was investigated in alkali electrolytes for the first time by using linear sweep voltammetry with rotating disk electrode (RDE). The oxygen reduction reaction (ORR) activities of these alkali iron phosphates are comparable to that of Pt/C system. The Tafel slope and electron transfer number of the alkali iron phosphates were calculated. The ORR activity of $NaFePO_4$ was found to be better than $KFePO_4$ and $FePO_4$. This work demonstrates alkali iron phosphates as alternate cost-effective, novel electrocatalysts for productive ORR activity in alkaline solution.

Keywords:$AFePO_4$, Electrocatalyst, Oxygen reduction reaction, Earth-abundant, crystal structure.

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DOI: https://dx.doi.org/10.5281/zenodo.1170682

Fabrication and Studies on Microstructure, XRD and Properties of Nano Copper Alloys

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ABSTRACT

Nano materials result from the grain size of the polycrystalline materials being reduced through different processing techniques. During the process dimensional change takes place on the order of nano materials corresponding to large increase in the volume fraction of grain boundaries. Most of the processing and consolidation challenges that have really hunted nanocrystalline materials are now totally understood. Recent advances in theoretical computation and experimental capabilities have allowed mechanical alloying in powder processing technique in solid state form using harder balls (Agate) in ball milling. Micro alloying can enhance the corrosion resistant properties (1) besides enhancement of mechanical properties. The following nano copper alloys have been synthesized through the special metallurgical technique and several characteristic properties of the materials are studied.

1. Cu-Zn-Pb
2. Cu-Zn-Al
3. Cu-Sn-Ag
4. Cu-Sn-Fe
5. Nano porous copper
6. Nano copper crystals

Mechanical properties of wire type nano materials are measured (Tensile Test). Electrical conductivity at ambient temperature and at different higher temperatures is measured. Small addition of metal oxides like Lanthanum (anti corrosion properties), Cerium (Grain reinforcement agent) (2) are very interesting in nano alloys. Stabilization of microstructure takes place during the synthesis with additives. High mechanical properties at elevated temperature and, increase of the strength of alloy is quite observable in nano copper alloys with additives like Al, Zn, Ag, Pb, etc. Additives are also useful in deoxidization process and purification of metal baths during the process of melting.

Key Words: Nano copper, Copper Alloys, Microstructure, Corrosion resistance, Mechanical Properties

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DOI: https://dx.doi.org/10.5281/zenodo.1167624

Magnetic Properties of $Pb_6Co_9(TeO_6)_5$ single crystal

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$Pb_6Co_9(TeO_6)_5$has a unique type ofmagnetic spin lattice structure, where the spin lattice consists of four different Co ions sites withdistorted octahedral coordination. DC magnetization measurements exhibits, a complex magnetic behavior, ferromagnetic transition (T_C) at ∼21.5 K. At lower magnetic fields, ZFC (Zero-fieldcooled) and and FC (field-cooled) curves show a broad hump at T_b∼10.8 K and a shoulder peakat T_s∼6.2 K below TC, which are suppressed in higher applied magnetic fields. AC susceptibilityand specific heat (CP) measurements also confirm the FM transition at low-temperature, however, there is no trace of peak observed except T_C. Remarkably, the negative Curie-Weiss constantreveals in H ||c, H ⊥c and powder sample at high temperatures, suggesting antiferromagnetic(AFM) interactions at high temperatures. The frustration factor, is found be 7.2 along H ||$c$while almost absent in H ⊥c and also reduced with applying higher magnetic fields. The large coercive curve (HC) observed (1.3 T) at 2 K applying magnetic field along H ||c, whereas linearmagnetization curve exhibits for H⊥c. These behaviors indicate the highly anisotropy nature ofpresent compound. The short-range magnetic spin correlation is present above T_C.

DOI: https://dx.doi.org/10.5281/zenodo.1170684

Nano-molar Ag ion detection using ZnS QDs in the UV-Vis technique without organic mediator

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Abstract

Ag shows large applications e.g. excellent electrical and thermal conductors, metal reflectors, anti-bacterial uses and in jewel industries. However, it is found to be hazardous and potent threat to health and environment [1]. The environmental protection agency has set maximum contaminant level for Ag at 0.1 mg/L (0.93 μM) and therefore it warrants to be detected at low concentration.

We report, for the first time, an ultra small amount of Ag^+ detection without using any organic component as mediator by a simple UV-Visible (UV-Vis) technique. Quantum dots of ZnS prepared in a soft chemical route are utilized for detection [2]. UV-Vis and photoluminescence measurements decipher quantum confinement effect and various defects in ZnS nanoparticles, respectively. Defect band in ZnS nanoparticles prominently appears at 400 – 550 nm in UV-Vis region and is used for Ag^+ detection in aqueous solution. This defect containing surfaces in ZnS allow the formation of insoluble precipitate of Ag_2S, which is confirmed using X-ray diffraction measurement. In consequence, total absorption of ZnS NPs is affected providing platform for quantitative estimation for Ag^+ detection for a wide range of concentrations starting from nM to mM. The process is also extended to toxic and heavy elements *e.g.* Pb, Hg and Cd and crucial role of solubility and selective nature of Ag-S interaction are highlighted.

Keywords: ZnS, quantun dots, UV-Vis spectroscopy, Ag, heavy metals

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DOI: https://dx.doi.org/10.5281/zenodo.1170686

Properties of RF magnetron sputtered SnO_2:CuO (50:50) thin films

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Abstract

Tin oxide (SnO_2) and copper oxide (CuO) are widely used TCOs. SnO_2 is a *n*-type semiconductor with wide energy gap of 3.7 eV. CuO is a *p*-type semiconductor with energy gap of 1.5 eV. Because of their unique electrical and optical properties, both SnO_2 and CuO have wide range of applications such as gas sensor(1), flat panel display(2), photo catalyst (3) etc. Thin films of SnO_2:CuO (50:50) were deposited on pre-cleaned quartz substrate using RF sputtering with different sputtering powers. The XRD analysis shows that the prepared films were amorphous in nature. The uniform morphological feature was realized from the HRSEM micrographs. The optical property studied by UV-Vis NIR spectrophotometer shows that the transmittance of the film decreases with increase in the sputtering power and the band gap decreases from 3.80 eV to 3.59 eV with increase in the sputtering power.

Keywords: Mixed oxide, thin films, physical properties

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DOI: https://dx.doi.org/10.5281/zenodo.1170688

Ferroelectric and Piezoelectric Properties of $(Ba_{0.95}Ca_{0.05})(Ti_{0.92}Zr_{0.04}Sn_{0.04})O_3$ Lead-Free Electroceramic

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Abstract

The lead-free $(Ba_{0.95}Ca_{0.05})(Ti_{0.92}Zr_{0.04}Sn_{0.04})O_3$ (BCZST) electroceramic was prepared by solid state reaction method; investigated ferroelectric and piezoelectric properties. The formation of perovskite structure without any secondary phase suggesting that Ca^{2+}, Sn^{4+} and Zr^{4+} well diffused in $BaTiO_3$ lattice to form a solid solution. The dense microstructure with an average grain size of 23.5 µm is observed having relative density ~ 95%. Temperature dependent dielectric measurement shows the dielectric maxima at Curie temperature, $T_c = 92\ ^{o}C$ with $\varepsilon_r = 8142$. Polarization measurement to an applied electric field exhibit the typical hysteresis loop with $P_r = 5.83\ \mu C/cm^2$ and $E_c = 2.45$ kV/cm, which confirms the ferroelectric nature of BCZST. The poled BCZST sample exhibits the direct piezoelectric coefficient $d_{33} = 296$ pC/N and converse piezoelectric coefficient $d_{33}^* = 268$ pm/V. The present BCZST ceramic with moderate ferroelectric and piezoelectric properties can be useful for developing the piezoelectric devices.

Keywords - Ferroelectric, Piezoelectric, $BaTiO_3$, Piezoelectric coefficient

DOI: https://dx.doi.org/10.5281/zenodo.1170690

Dielectric, Ferroelectric, and Piezoelectric Properties of Ca^{2+}/ Sn^{4+} modified $(Ba_{0.97}Ca_{0.03}Ti_{0.97}Sn_{0.03})O_3$ Lead-Free Electroceramic

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Abstract

$BaTiO_3$ based lead-free electroceramic modified by Ca^{2+}/Sn^{4+} i.e. $Ba_{0.97}Ca_{0.03}Ti_{0.97}Sn_{0.03}O_3$ was synthesized using solid-state reaction method; investigated dielectric, ferroelectric and piezoelectric properties. The structural analysis shows that the formation of perovskite structure with tetragonal crystal lattice symmetry having *P4mm* space group. The microstructural observation reveals the dense microstructure having defined grain boundaries to grains with an average grain size ~ 38μm and the relative density of ~ *98 %*. The temperature dependent dielectric measurements reveal the dielectric maxima i.e. Curie temperature (T_C) at $115\ ^oC$ having dielectric constant $\varepsilon_r \sim 12857$. The ferroelectric nature of the sample was confirmed from the electric field induced polarization-electric field (P-E) hysteresis loop measurement having $P_r = 5.19\ \mu C/cm^2$, $E_c = 2.14$ kV/cm. The poled $Ba_{0.97}Ca_{0.03}Ti_{0.97}Sn_{0.03}O_3$ exhibit the piezoelectric charge coefficient of 280 pC/N. The present study gives an insight on the stabilization of Tc for $BaTiO_3$ based lead-free ceramics by Ca^{2+} and Sn^{4+} modification.

Keywords – Lead-free piezoelectric, $BaTiO_3$, Dielectric constant, piezoelectric coefficient.

DOI: https://dx.doi.org/10.5281/zenodo.1170692

Magnetostrictive behavior of $NiFe_2O_4$ synthesized by modified solution combustion method

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Abstract

$NiFe_2O_4$ magnetic nanoparticles prepared at 600 ^{o}C by modified glycine/acrylic acid assisted solution combustion route; investigated its structural and magnetic properties. The phase formation and crystallographic information was analyzed by X-ray diffraction technique with Rietveld refinement. The microstructure reveals the formation of agglomerated particles due to non uniform temperature gradient during redox reaction, which is a typical characteristic of combustion synthesis. The magnetic parameters viz. saturation magnetization is 22.874 emu/g, retentivity 4.4325 emu/g, and coercivity 138.30 Oe is observed from magnetic hysteresis loop. Fourier transform infrared spectroscopy reveals the presence of octahedral and tetrahedral absorption bands which evidences the formation of spinel lattice. The magnetostrictive coefficient (λ_{11}) measured when magnetic field is applied parallel to sample and surface of the strain gauge; observed λ_{11max} $NiFe_2O_4$ is11 ppm. The experimental design for studying the magnetostrictive properties of materials is discussed in this paper with case study of $NiFe_2O_4$.

Keywords: Ferrite, combustion synthesis, magnetostriction, spinel structure.

DOI: https://dx.doi.org/10.5281/zenodo.1170694

Radio Frequency Magnetron Sputtered CuO:Al_2O_3 Thin Films for Gas Sensing Applications

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Abstract

In recent years, mixed metal oxide thin films have been greatly attracting the attention of the material science community because of their potential exploitation in various applications (1). Mixed CuO and Al_2O_3 thin films have been explored in several applications, yet their use in gas sensing field is unknown. We report the preparation of CuO:Al_2O_3 (50:50) thin film on quartz glass substrate by radio frequency magnetron sputtering technique with RF powers of 200 and 300 W at room temperature. X-ray diffraction study showed the deposited films were amorphous in nature. The average transmittance of CuO:Al_2O_3 (50:50) films in the visible region is around 80-90%. The RF power induced variation in energy band gap of 3.92 to 4.18 eV was observed. The CuO:Al_2O_3 (50:50) film showed good selective response to NH_3 gas with very high sensing response of 80.75 (10 ppm NH_3) at room temperature.

Keywords: Aluminium oxide, Copper oxide, Thin film, RF Sputtering, Gas sensor

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DOI: https://dx.doi.org/10.5281/zenodo.1170698

Tunable Competition and Possible Coexistence of Magneto-Electric Phases in a Charge Ordered Manganite

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Abstract

The cross control of magnetization (electric polarization) by an external electric (magnetic) field and coupling between them in single phase material yields a new and exciting fields (1). To enhance the magneto-electric (ME) signal, effective control of a phase competition has recently been revealed as a promising approach. Herein, we report the magnetic field (H) control of the distinct ME phases in a charge ordered magnet $Pr_{0.75}Na_{0.25}MnO_3$, in which an antiferromagnetic (AFM) phase is competing with a ferromagnetic (FM) phase(2,3). The H dependent dielectric behavior is highly correlated but in contrast to their resistivity (2). The variation of ε with H is intrinsically associated with the coexisting phases of contrasting order. However, the ground state is FM. Using suitable experimental protocol the magnetic phases as well as electronic phases can be tuned effectively at low-H vis-à-vis to enhance the ME signal. The apparent change in ME signal in accordance with macroscopic phase competition are modelled through Maxwell's dynamical theory (4, 5).

Keywords: Charge ordering, Manganite, Competing phase, Magnetoelectric

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DOI: https://dx.doi.org/10.5281/zenodo.1170700

Nanochain of BiFeO3 and Bi2Fe4O9 Prepared by hydrothermal method and study of their magnetic properties

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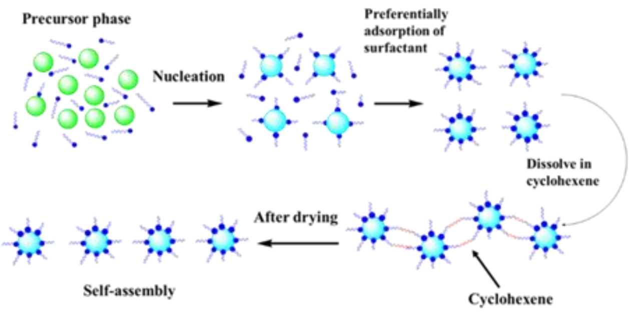
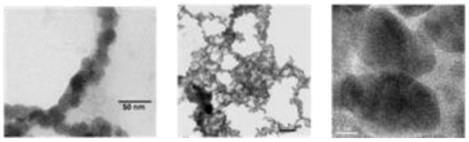
Abstract:

Synthesis of self-assembled magnetic nanochains is found to be very promising because of their distinctive optical, electrochemical and magnetic properties. They can be used in microchemical sensor, magnetic switching, DNA separation etc. Here 18-carbon chain fatty-acid is used as surfactant. We have synthesized BiFeO3 and Bi2Fe4O9 nanochains. The morphology, chemical composition, phase purity and crystal structure of the as-prepared samples were determined by TEM, EDX and XRD respectively. The nano chains are composed of spherical particles of size 20-30 nm. Length of the nanochains varies from few tens of nanometres to even few micrometres. We have measured the room temperature magnetic properties such as magnetization at 1.5 Tesla, remnant magnetic moment, coercivity etc. We have noticed differences in the magnetic properties between those of isolated nanoparticles and their self-assembled patterns. The results appear to be promising for tuning the multiferroic properties by tailoring different self-assembled patterns of the nanoscale particles.





Keywords: Multiferroics, Self-assembly, Enhance-magnetization

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DOI: https://dx.doi.org/10.5281/zenodo.1170702

Synthesis of Nickel Cobalt MangneseSulphide (NCMS) by electrodeposition for Supercapacitor applications

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Abstract:

Nickel Cobalt MangneseSulphide (NCMS) nanostructures have been prepared by simple and cost effective electrodeposition technique on Nickel (Ni) foam.The electrochemical measurements were investigated by using cyclic voltammetry andgalvonostatic charging discharging. The large surface area of NCMS leads to high specific capacitance of 2581 F/g at a scan rate of 1mV/s by CV measurements and a capacitance of 5008.08 F/g by GCD measurements. The material shows an excellent stability of 57% at 3000 cycles at a current density of 100 A/g. Hence the NCMS nanostructured material demonstrate the application in efficient energy storage applications at high current density.

Keywords: Nickel Cobalt MangneseSulphide (NCMS), electrochemical measurements, energy storage applications.

DOI: https://dx.doi.org/10.5281/zenodo.1170704

Photo physical, photodegradation and biological studies of synthesized porphyrins (P1, P2) and metallo porphyrins (Pz1 Pz2)

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Porphyrins and metalloporphyrins were formulated by linking phenothiazine and methoxy substituted phenyl ring and characterized by ^{1}H and ^{13}C mass spectra. The photo physical properties have been investigated by UV –Vis absorption, steady state fluorescence spectroscopy and cyclic voltammetry measurements. The photocatalytic activity of these materials was evaluated by UV-Vis spectroscopy for the degradation of congored under sunlight radiation. Antibacterial activities of the prepared samples were screened agai2.54nst Gram positive and Gram negative bacteria by measuring the zone of inhibition. Antioxidant activities were performed of porphyrins and metalloporphyrins for DPPH assay. In-vitro lung cancer (A549) activity of synthesized samples was carried out using MTT assay.

Keywords: Porphyrins, photo physical properties, antibacterial, antioxidant and anticancer activities.

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DOI: https://dx.doi.org/10.5281/zenodo.1167628

INFLUENCE OF Zn CONCENTRATION ON THE PROPERTIES OF La_2O_3 NANOSTRUCTURES

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ABSTRACT

Lanthanum oxide (La_2O_3) nanoparticles were synthesized by a simple sol gel method. Lanthanum nitrate, Zinc nitrate, Citric acid and double distilled water are used as starting materials. The samples with different Zn concentrations namely 0.1 and 0.2 mol were prepared with a reaction time of 3 & 6 hrs. The samples were calcinated at a temperature of 500°C for 2 hour. The as-prepared and calcinated samples have been subjected to various characterizations. The phase and structure of the samples have been identified by using X-ray diffraction. The morphology of the synthesized particles has been investigated by a scanning electron microscope (SEM). The SEM images of equal concentration samples (0.01 mol) show spherical structures. The FTIR spectra show the presence of different functional group present in the synthesized Nanoparticles. The absorbance spectra have been recorded in the UV-Visible region and analyzed.

Key words: La_2O_3:Zn; Band gap; SEM

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DOI: https://dx.doi.org/10.5281/zenodo.1170706

ZnO-NiOhetrostructure: synthesis, properties and performanceas photocatalystfor degradation of organic pollutants

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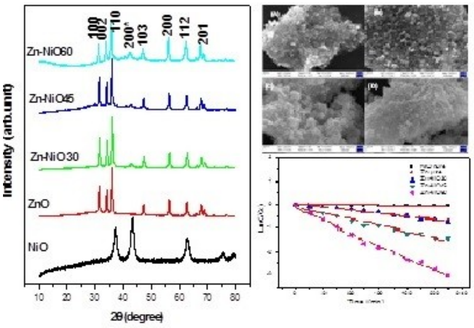
Abstract

Zinc oxide (ZnO) basedmaterials has attracted much interest in the field of photocatalytic degradation of organic pollutants from waste water. This is due to its high photosensitivity, sustainable band gap, low cost and environmental compatibility [1]. In the present work,ZnO-NiOnanocomposites with different NiO concentrations were synthesized by sonochemical method using zinc acetate (Zn(CH3COO)2), nickel acetate and sodium hydroxide (NaOH) as starting materials. X-ray diffraction (XRD) analysis confirm the hexagonal wurtzite phase for ZnO and cubic phase for NiO. Scanning electron microscopy (SEM) and elemental dot mapping reveals the formation of ZnO-NiO heterostructures with uniform distribution of both components. The photocatalytic performance of the samples were investigated using methylene blue as a model dye under visible (75W Mercury vapor lamp) irradiation. ZnO-NiO heterostructures with different NiO concentration shows better photocatalytic activity than individual metaloxides revealing synergetic effect. This is because of the charge transfer that could happen between the p-type and n-type oxides enhancing the photocatalutic activity [2].



Keywords:**Nanocomposite, hetrostructure,Photocatalyst,Sonochemical synthesis**

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DOI: https://dx.doi.org/10.5281/zenodo.1170709

Performance of reduced graphene oxide (RGO) as active material for electrochemical supercapacitor applications

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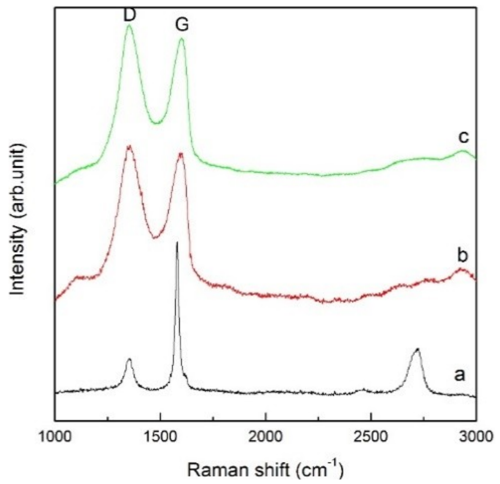
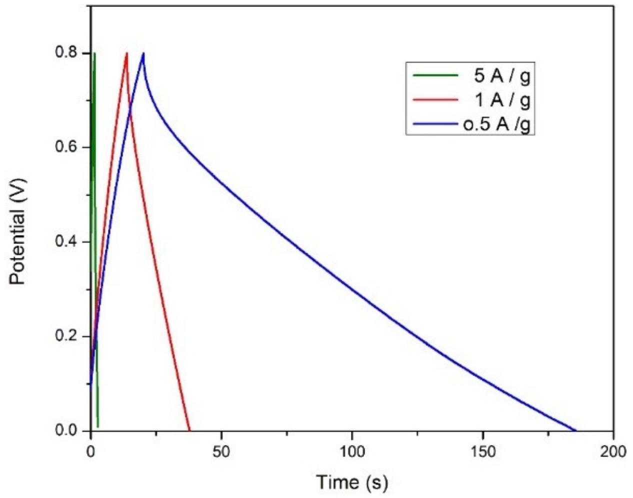
Abstract

Beyond pristine graphene, reduced graphene oxide with a few layers also find important applications in many areas including electrochemical devices. In this context, the reduction of electrically insulating graphite oxide (GO) to reduced graphene oxide (RGO) is important.GO has wide range of oxygen functionalities; the reduction of GO significantly removes these oxygen functional groups. In the present work GO is prepared by modified hummers method and it is reduced using hydrazine [1]. The chemical and structural properties were analyzed by TGA, XRD, SEM and Raman spectroscopy. The structural changes occurred during the transition from GO to RGO is reflected in the Raman spectra.The electrochemical performance of samples were studied using cyclic voltammetry (CV) and galvanostatic charge – discharge (CD) techniques. CD measurements RGO yields a specific capacitance of 232 F/g at 0.5 A/g.





Keywords: **Reduced grphene oxide, modified Hummers method, Specific capacitance**

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DOI: https://dx.doi.org/10.5281/zenodo.1170713

Exploration of K-ion Intercalation in Iron-Based Mixed-Polyanion Material

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Abstract:

Li-ion battery (LIB) innovation has demonstrated predominance in powering portable electronics and electric vehicles, it remains questionable whether the limited resources for many of the metals in LIBs can satisfy the demands from the large-scale application in grid-level storage. This uncertainty has generated broad research interest into cost-effective alternatives. In this context, Na-ion batteries (NIBs) have been examined as a promising option because of the abundance of Na and the similar chemistries of Li system. However, there are two fundamental natural issues associated with NIB technology (i) the higher standard redox potential of Na/Na^+ usually translates into a lower working voltage than Li^+ and (ii) graphite, a conventional anode for LIBs, cannot reversibly intercalate Na ions, instead requiring the use of hard carbon anodes.Thus, K-ion batteries (KIBs) with abundant K resources may be preferable as the standard redox potential of K/K^+ is lower than that of Na/Na^+, and graphite can store and release K ions. Keeping these issues in mind,we have investigated K-ion intercalating properties of Iron-based mixed-polyanion $Na_4Fe_3(PO_4)_2P_2O_7$. The cathode material was prepared by solution combustion synthesis using ascorbic acid as reducing agent and fuel. It has a 3D intercalating structure and the K-ion cell with $Na_4Fe_3(PO_4)_2P_2O_7$ cathode showed first discharge capacity of 118 mAh g^{-1} (92 % of its theoretical capacity) and excellent capacity retention with good cycling stability (100 cycles). The work demonstrates the capability of the material as a high-performance cathode for K-ion batteries due to its multiple K-ion sites in the structure.

Keywords: mixed-polyanion cathode, $Na_4Fe_3(PO_4)_2P_2O_7$, solution combustion synthesis, potassium-ion battery, Capacity

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DOI: https://dx.doi.org/10.5281/zenodo.1170748

Effect Of Ag And Na On Electrical Properties In LCSMO CMR Manganites

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Abstract.

Synthesis and characterization of colossal magnetoresistance (CMR) materials have been a subject of scientific research due to the unique transport, magnetotransport, and magnetic properties. The single phase polycrystalline $La_{0.7}Ca_{0.1}Sr_{0.1}M_{0.1}MnO_3$ (LCSMO) (M=Ag and Na) samples prepared using the nitrate route method. The temperature dependent electrical resistivity ρ(T) of samples shows two transition peaks, a typical characteristics of Ag doped lanthanum based manganites while Na doped manganites exhibit one transition peak. In the high temperature range, the VRH model is found to simulate the resistivity behavior marginally better as compared to the small polaron model. The anomalous low temperature behavior is explained in terms of a model which combines electron-electron scattering and weak localization. The study of magneto transport behavior in both samples revealed enhanced negative MR of about 55 % in the low temperature range due to the spin polarized tunneling across the grain boundaries. Significant MR at room temperature can be exploited for magnetic sensing applications (1, 2).

Keywords: Nano-crystalline manganites, colossal magneto resistivity, metal to insulator transition, broad magnetoresistance, Weak localization.

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DOI: https://dx.doi.org/10.5281/zenodo.1170751

Investigation on Structural, Transport, Magnetic and Magneto caloric properties of Cu substitution in CoMnGe alloys

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Abstract

We investigate structure, transport, magnetic and magnetocaloric effect in $\mathrm{Mn}Co_{1-x}Cu_xGe$ (x = 0, 0.3, 0.7) intermetallic alloys. The non-magnetic (Cu) element is positioned at Co site, which results drastic change in the crystallographic structure (Orthorhombic-Hexagonal) and exhibits metal-insulator behavior. The magneto-structural transition reduces and changes from First (AFM-FM) to Second (FM-PM)) order with Cu substitution. Giant MCE is observed near RT (307 K) for parent sample and decreases towards lower temperatures for Cu doped samples. The change in magnetic entropy (ΔS_M) decreases with increasing Cu substitution. Refrigeration capacities (RC) linearly increase with magnetic field for all samples and decreases with Cu doping. The order of transition is confirmed for x=0.2, 0.4, 0.6 alloys by the analysis of critical exponents via modified Arrott plots and the Kouvel Fisher method. The calculation of Landau coefficients, Spontaneous magnetizations and local exponent from isothermal curves will be discussed in details manner.

Keywords: MnCoGe, Metal-Insulator, Magnetic refrigeration, Critical exponents.

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Acknowledgement:

The author U.D acknowledges for funding to SERB- National Post Doctoral fellowship (PDF/2016/000412).

DOI: https://dx.doi.org/10.5281/zenodo.1170753

Observation of Itinerant antiferromagnetism in Y-substituted $CeNiGe_2$

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We investigate the results of magnetization and resistivity studies on Y substituted heavy fermionic system $CeNiGe_2$. Investigations are carried out on the compounds $CeNiGe_2$, $Ce_{0.9}Y_{0.1}NiGe_2$, $Ce_{0.8}Y_{0.2}NiGe_2$ and $Ce_{0.6}Y_{0.4}NiGe_2$. In $CeNiGe_2$, it is observed that a fraction of delocalized spin coexists with localized spins. With the increase Y concentration, the antiferromagnetic transition temperature decreases while itinerant moments increases. It is also noted that resistivity increases across the series. This observation points that with the increase in Y-substitution, the decrease of resistivity below ordering temperature is suppressed indicating that the itinerancy increases leading to enhanced scattering. Thus site dilution of Ce results in the observation of itinerant antiferromagnetic behavior in these compounds.

Keywords: Intermetallic compounds, charge carriers.

PACS: 71.20.Lp, 72.20.Jv,

DOI: https://dx.doi.org/10.5281/zenodo.1170755

Synthesis, structure and dielectric properties of giant dielectric $Ti_{1-x}(Al_{0.5}Nb_{0.5})_xO_2$ (x=0.01,0.05,0.1) ceramics

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Abstract

Capacitors have an advantage over batteries with respect to the endurance for charge - discharge cycling and power density. Capacitors can replace Li-ion batteries if energy density can be increased significantly. Use of electric double-layer capacitor (EDLC) is restricted because of the relatively low energy density of EDLC in comparison with lithium ion battery and the leakage of liquid electrolyte from packages. The capacitance density of multi-layered ceramic capacitors (MLCCs) has been increased one million but $BaTiO_3$ based material exhibits poor temperature or frequency stability. In view of that urgent need, the search for materials with giant permittivity (GP, $\varepsilon' = 10^4$–10^5 in a radio frequency range) has been attracting considerable attention for many years due to its very high capacitance and energy density. Very recently, GP with low dielectric loss was reported in (In, Nb) co-doped rutile TiO_2 polycrystalline ceramics [1]. However, it is not economic to use indium oxide due to its high cost. The colossal permittivity is retained with low dielectric loss by replacing indium oxide by cheap and abundant aluminium oxide [2].

Here, we investigated the dielectric properties of $Ti_{1-x}(Al_{0.5}Nb_{0.5})_xO_2$ [x=0.01,0.05,0.1]ceramics prepared by the solid-state method at various calcination and sintering temperatures. Both calcination and sintering temperature have significant effect on phase formation, density, grain size, which are related to dielectric property. The calcination temperature has a great influence on the grain boundary, and that modifies the dielectric property. Impedance spectroscopy was used to explain the mechanism of giant permittivity.

Keywords: **Rutile–TiO_2, Giant dielectric permittivity, Sintering, Impedance spectroscopy**

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DOI: https://dx.doi.org/10.5281/zenodo.1170759

$LiCeWO_4)_2$ Polymorphs: A Novel Anode Material for Lithium-Ion Batteries Crystal Structure Correlation via Neutron Diffraction Study

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Abstract

Rare earth oxide materials are multifunctional disordered materials widely studied for laser media optoelectronics[1-3]. Among various rare earth oxides, Li*RE*$(WO_4)_2$ (*RE*=lanthanides) exist in a wide variety of crystal systems and also exhibits polymorphism[4, 5]. More recently these materials are also been used in lithium ion battery applications and shown interesting electrochemical behavior[6, 7].

In the present study, polymorphs of Li*Ce*$(WO_4)_2$ were synthesized via solgel method and Rietveld refinements were carried out using high temperature Neutron diffraction data collected at ANSTO. Further, Li*Ce*$(WO_4)_2$ polymorphs were examined using galvanostatic measurements as anode materials for lithium ion batteries for the first time. To the best of our knowledge this is the first study elucidating synthesis, detailed crystal structure analysis, structural phase transitions and the electrochemical properties of Li*Ce*$(WO_4)_2$ polymorphs. Hence, the insights of our study would be helpful for scientific community to achieve better results from these materials with modifications or surface coating in future studies.

Key words: Polymorphs, Phase transitions, Neutron diffraction and Anode battery material.

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DOI: https://dx.doi.org/10.5281/zenodo.1170764

The high strain rate deformation of a high-strength, high-toughness 10Ni-0.1C steel

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Abstract

We have characterized the propensity for adiabatic shear band formation under dynamic deformation conditions in an ultra-high strength (1.1GPa) 10Ni steel and demonstrated that in spite of its outstanding static toughness, this steel is highly prone to shear localization and failure.

Specifically, microstructural evolution during deformation of a Fe-10 Ni-0.1C-Cr,Mo,V steel was examined. In the high-strength condition (influenced by tempering parameters), the steel has a lath martensite microstructure with a mean lath size of ~60 nm, and MC carbides dispersed in it with a mean size of ~20 nm. During compressive dynamic deformation using a split Hopkinson bar (strain rates of 1000 to 4000 per second), depending on strain and strain rate, shear localization occurs and is accompanied by an optically visible shear band (~20 micrometers wide). In the situation where the localization process is in its early stages (lower rates, lower global height strains, or both), the microstructure shows severe local deformation within the band but the initial microstructure is still discernible.

DOI: https://dx.doi.org/10.5281/zenodo.1170766

Solid state synthesis of rare earth orthochromite $La_{(1-x)}Sm_xCrO_3$ nanoperovskite with its dopant concentrations

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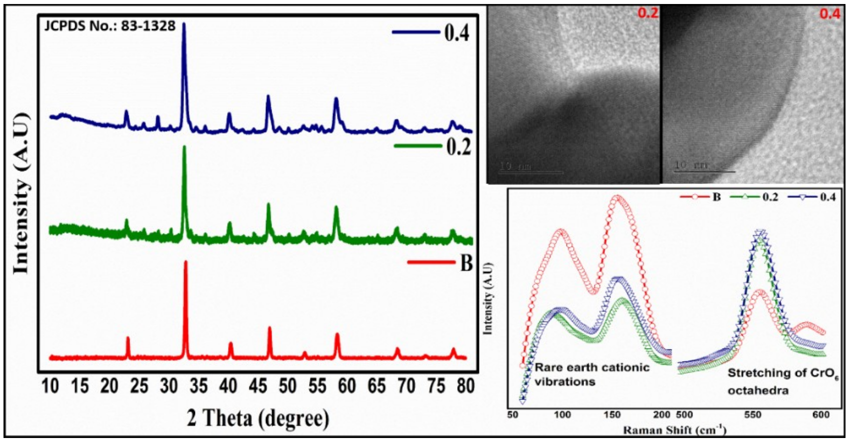
[#] *Equally contributed authors*

Abstract:

The systematic solid state synthesis and investigation of rare earth orthochromites $La_{(1-x)}Sm_xCrO_3$ (x ≈ 0, 0.2 and 0.4) have been reported. The polycrystalline $La_{(1-x)}Sm_xCrO_3$ (LSCO) nanoperovskite materials were known to be in a single phase orthorhombic crystal system and maintained its inherent octahedral distortions for the observed tolerance factor ($0.8 \leq T \geq 0.9$). Phonon Raman modes were assigned and correlated with the structure of synthesized LSCO nanoperovskite. Relative doping of samarium results in blue shift emission around $\lambda \approx 3$ nm from that of parent $LaCrO_3$ nanoperovskite. The change in respective properties of synthesized LSCO nanoperovskite is mostly attributed to the coulombic interaction with respect to their relative ionic radii. Elemental analysis confirms the presence of stoichiometric dopants for respective LSCO orthochromites. The finer particles tend to aggregate with adecrease of samarium dopants onto the lattice sites of $LaCrO_3$ nanoperovskite as inferred from microscopy studies. Magnetization analysis shows that feeble antiferromagnetism exhibited by parent has been observabledue to the effective introduction of increasing samarium dopants.



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DOI: https://dx.doi.org/10.5281/zenodo.1167634

K-Br system under pressure: synthesis of unconventional stoichiometric compounds

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Abstract:

The search and synthesis of unconventional stoichiometric compounds has become one of the most active areas of high pressure research in recent times. Although several such compounds have been predicted theoretically, very few have been realized experimentally. The notable examples of such compounds are $NaCl_3$, Na_3Cl, lithium polyhydrides and KCl_3. The experimental realization of more such compounds will enhance our scientific knowledge of the related solid state chemistry. In the present study we report the synthesis of two new stoichiometric compounds, namely KBr_3 and KBr_5 at high pressures in the K-Br system. Two independent experimental techniques namely, diamond anvil cell (DAC) based Raman spectroscopy and x-ray diffraction measurements were employed to detect and confirm the formation of the new compounds. A room temperature chemical reaction between KBr and Br_2 resulted in the formation of an orthorhombic KBr_3 (*SG: Pnma*) at ~ 2.0 GPa. Further compression lead to the formation of a monoclinic KBr_5 (*SG:* $P2_1$) at ~ 6.0 GPa. This is the first ever experimental synthesis of a 1:5 stoichiometric compound in the alkali halogen system. Formation of KBr_5 was accompanied by an anomalously large pressure (> 2GPa) increase inside the sample chamber and it remains stable up to the highest pressure (24 GPa) of our study. Furthermore, high-pressure (14–20 GPa) and high-temperature (> 1500 K) laser heating experiments showed the decomposition of KBr_5 into a trigonal KBr_3 (*SG: P-3C1*) and Br_2 with a large volume reduction. First-principles structural searches using the USPEX code in combination with VASP code were carried out to solve the composition and related crystal structures.

Keywords: High Pressure Synthesis, x-ray diffraction, Raman spectroscopy, Laser heating

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DOI: https://dx.doi.org/10.5281/zenodo.1170768

Comparison studies on morphology and optical properties of thin film CdS by chemical bath deposition and spin coating technique

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Abstract

The thin film of cadmium sulfide (CdS) was deposited on a soda lime glass substrate by chemical bath deposition (CBD) and spin coating technique. In CBD technique, the deposition was performed at 60°C, 70°C, 80°C and 90°C during various deposition times (30, 60, 90 and 120 min). In spin coating technique, CdS film was deposited at 1600 rpm, 1800 rpm, 2000 rpm, 2200 rpm and speeds of 2500 rpm. The morphological, chemical composition and optical properties of CdS film were investigated for both techniques using the scanning electron microscope (SEM), energy dispersive X-ray spectroscopy (EDX) and the UV-Vis-NIR spectrophotometer. From these investigations, an appropriate CdS film was obtained which is related to uniform deposition, the equal contribution of the atomic percentage Cd and S, band gap value ~2.42 eV, high transmittance and low resistivity. Such optimized CdS film will perform as an n-type window layer for thin film solar cell.

Keywords: CdS, chemical bath deposition, spin coating, morphological properties.

DOI: https://dx.doi.org/10.5281/zenodo.1170770

Investigation of structural and magnetic properties of $RBaFeMnO_6$ (R = Nd, Sm) double perovskites

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Abstract

The polycrystalline $RBaFeMnO_6$ (R=Nd and Sm) double perovskites have been synthesized using nitrate-glycine auto-combustion synthesis method followed by single step calcination process [1]. The room temperature powder X-ray diffraction patterns reveal that synthesized samples crystallize into an ideal cubic perovskite crystal structure with space group Pm-3m. The structural parameters have been refined by Rietveld analysis method [2] using FullProf Suite software [3]. The value of lattice constant "a" decreases from a=3.894Å for NBFMO to a=3.889Å for SBFMO due to smaller ionic radius of Sm (0.958Å) than Nd (0.983Å) [4]. The temperature dependent magnetization M(T) curves reveal that these samples undergo paramagnetic to antiferromagnetic phase transition at Neel temperature T_N. The field dependence of magnetization M(H) measurement shows coexistence of ferromagnetic and antiferromagnetic fractions at low temperature (5K). The UV-Vis spectroscopy measurement reveals high energy band gap between conduction band and valence band of the order of E_g~6eV.

"Keywords: X-Ray Diffraction; Auto-Combustion Method; Rietveld Refinement; FullProf Suite; Energy Band Gap."

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DOI: https://dx.doi.org/10.5281/zenodo.1170772

Upper critical field analysis of NbN superconductor

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Abstract

Thin film Niobium Nitrides(NbN) deposited by reactive sputtering have been characterized. The NbN films with cubic fcc B1 structure has a maximum T_c of 13.4K. The upper critical field $B_{c2}(0)$ for of these set of thin films has been calculated using GLAG theory with a maximum of 72T for one of the films, while other films show $B_{c2}(0)$ greater than 40T[1]. In the present work, these results have been analysed using Werthamer Helfand and Hohenberg (WHH) theory for disordered metals in the dirty limit. The variation of $B_{c2}(T)$ with T has been fitted to the WHH equation with paramagnetic limiting parameter α and spin-orbit parameter λ_{so}. The results indicate the importance of both α and λ_{so} in understanding the Upper critical field and will be presented.

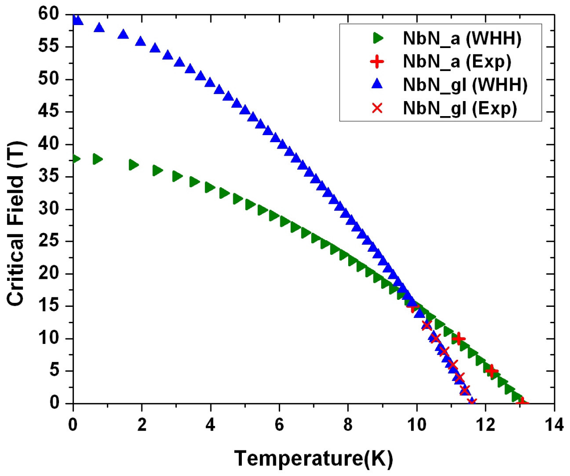

Fig.1. Dependence of experimentally measured Bc2(T) and calculated Bc2(T) with temperature for two typical NbN thin films.

Key words: DC sputtering, Niobium Nitride, Superconductivity, Upper critical field, Werthamer, Helfand and Hohenberg theory.

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Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials

Defect studies on chemically synthesized FeCo by positron lifetime spectroscopy

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Abstract

FeCo alloys exhibit B2 type ordered and A2 type disordered structure whose magnetic and mechanical properties are different. Positron lifetime spectroscopy (PAS) was undertaken for the chemically synthesized FeCo samples and compared with Fe, Co and annealed FeCo. PAS of the asprepared sample resulted in two short lived lifetime components and two long lived lifetime components in the ns region. The shorter lifetime components are attributed to the interfaces and cluster vacancies respectively. The longer lifetime components originate from pick-off annihilation of orthopositronium (o-Ps) in the small and large voids and its annihilation at larger voids due to the flower like morphology. The disordered FeCo transforms to the ordered form on annealing at 700 °C. The studies suggest that FeCo alloys synthesized through chemical methods could also produce porous structure with properties different from the bulk.

Keywords: Positron annihilation, magnetic nanoparticles, soft magnetic materials

DOI: https://dx.doi.org/10.5281/zenodo.1170778

Synthesis and DFT studies of a novel ESIPT 2-(2′-Hydroxyphenyl)-1*H*-benzimidazole derivative

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Abstract

Molecules having excited state intramolecular proton transfer (ESIPT) show characteristic properties like large stokes shift and dual fluorescence emission. Such molecules are used in various fields as lasers, fluorescence probes, sensors, and optical devices. 2,(2′-hydroxyphenyl)-1H-benzimidazole (HBL) and its analogues are a family of widely studied ESIPT fluorophores. In the present work, we have tuned HBL by another proton donating site to further enhance its Stokes shift. The novel HBL derivative, 2-(1H-benzimidazol-2-yl)-4-(2-hydroxybenzylideneamino) phenol, was synthesized and the structure was confirmed using ^{1}H NMR spectroscopy. Feasibility of proton transfer was elucidated by potential energy scan (PES) in ground state on a pair of oxygen-hydrogen using Density Functional Theory (DFT). The calculations carried out using long range corrected functional CAM-B3LYP and 6-31 g(d, p) basis set in presence of methanol environment adopted by PCM show least probability of proton transfer in the ground state. However, back proton transfer from excited state to ground state can happen easily. UV-Vis absorption spectrum obtained by the same method shows three peaks at 287, 313 and 331 nm, due to π-π* transition of benzene ring, cis-enol and trans-enol conformations, respectively.

Key words: ESIPT, DFT, PES

DOI: https://dx.doi.org/10.5281/zenodo.1170782

Investigation of magnetic properties of a cluster-glass system Dy_5PdNi

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Abstract

Rare earth intermetallic compounds of the form R_5Pd_2 are extensive investigated as these materials have complex magnetic behavior [1-2]. Dy_5Pd_2 belongs to this family and exhibits glassy magnetic state along with magnetocaloric effect (MCE) [2]. Ni substitution at the Pd site can be an effective approach to tune the magnetic properties of Dy_5Pd_2. Therefore, investigations were carried out on the compound Dy_5PdNi. DC magnetization shows a peak at 38 K and below this temperature glass-like magnetic behavior had been observed. Inverse susceptibility was fitted with Curie-Weiss law, which deviate from straight line below 90 K indicating that the short range magnetic ordering persist upto 90 K. Dy_5PdNi exhibits the irreversible behaviour at ~ 38 K when measured under the zero field cooled (ZFC) and field cooled (FC) protocols. With increasing field, this irreversibility temperature is decreased indicating the presence of glass-like magnetic state. Heat capacity results do not show any sharp peak, which supports, the absence of long range magnetic ordering in this compound. Ac susceptibility measurements show a shift in peak temperature with frequency Mydosh parameter ($\delta T_f = [\Delta T_f/(T_f(\Delta log f)$, for this compound was found to be around 0.025. Such value is noted for other compounds showing cluster glass behaviour implying that the observed glassy phase in this compound is cluster glass-like. In this compound, both conventional and inverse MCE is observed. The maximum value of the magnetic entropy change for a field change of 70 kOe was around 8.85 J/kg-K (at 55K) which is significant, indicating that Dy_5PdNi can be a good magnetocaloric material.

Keywords: Intermetallic compounds, Rare earth metal and alloy, Magnetic materials and magnetocaloric effect.

PACS: 71.20.Lp, 71.20.Eh, 75.30.Sg

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DOI: https://dx.doi.org/10.5281/zenodo.1170784

Synthesis and characterization of high curie temperature piezoelectric ceramics $BaTiNb_2O_8$

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Abstract

In recent years, there has been continued interest in high Curie temperature piezoelectric ceramics due to their stability in harsh environment applications such as aerospace and geological exploration. We present the x-ray diffraction, dielectric measurements and polarization-electric field hysteresis studies on new high Curie temperature piezoelectric $BaTiNb_2O_8$ ceramic synthesized by solid state route. The Powder x-ray diffraction reveals that the compound $BaTiNb_2O_8$ shows triclinic structure with space group P1. BTNO ceramic shows ferroelectric phase transition at very high Curie temperature $T_c = 468$ °C.

“Keywords: X-ray diffraction; Piezoelectric; Dielectric; SEM; EDS”.

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DOI: https://dx.doi.org/10.5281/zenodo.1170788

In-situ TiO_2/rGO Nanocomposites for CO Detection

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Abstract

TiO_2 is a well-known wide band gap semiconducting material for gas sensing applications owing to its high temperature stability, chemical stability and high catalytic behavior. However, its low electrical conductivity behavior became an impediment for its practical execution in chemiresistive / conductometric gas sensor (1). Graphene is a two-dimensional zero band gap layered structure which exhibits remarkable electron mobility at the room temperature. Despite, inadequate adsorption characteristics towards gas molecules is a restriction for gas sensing (2, 3). In order to enhance the sensing abilities, the hybridization of TiO_2 and Graphene seems to be an efficient method (4). In the current work, graphene oxide (GO) was synthesized through electrochemical exfoliation method. The TiO_2/rGO nanocomposites were prepared *In-situ* by hydrothermal synthesis using $TiCl_3$, ammonia and GO (5). XRD and SEM were performed for the microstructural and phase evolution. The sensing properties of TiO_2/rGO composite were investigated in CO environment.

Keywords: TiO_2 Gas sensors, CO detection, TiO_2/rGO composites.

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DOI: https://dx.doi.org/10.5281/zenodo.1170790

Flexible rGO-CB@Fe_3O_4/polydimethylsiloxane Composites for Electromagnetic Interference Shielding

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Abstract

Addressing the off-shoot of electromagnetic-interference, conducting polymer nanocomposites represent a novel class of materials that possess unique combination of electrical, dielectric, magnetic and mechanical properties which are useful for the suppression of electromagnetic noises. However, incorporation of various dielectric or magnetic fillers within polymer matrices without losing flexibility is a challenge. In the present work, we have investigated the effect of simultanious incorporation of carbonatious fillers and magnetic particles into the shielding effectivness (SE) of single layer silicon rubber (polydimethylsiloxane). We choose carbon-black as main filler since it strengthens the rubber as-well-as modifies the electrical conductivity and dielectric permittivity of the composite. Both conductivity and SE of the composite was progressively improved with CB addition, 2-20 wt%, and attained SE ≥20 dB in the frquency range of 8-12 GHz, while maintaining the flexibility. Further improvement in conductivity and mechanical properties were achieved by using r-graphene oxide/CB hybrid filler. In addition, we also investigated the effect of ferromagnetic phase (Fe_3O_4) along with CB/silicon rubber composite. The hybride structure shows excelent shielding perfomance orginates from the combined effect of dielectric loss and magnetic loss. The complex dielectric permittivity and permeability were also determined from the measured scattering parameters. The composites possess moderate polarization and magnetization alongwith good conductivity due to the combined effect of multi-fillers. The hybrid structure was also characterized by various techniques such as XRD, SEM, IR, and dielectric measurements. In short, the synegetic effect of multiple fillers suggesting new pathways for designing modern light weight shielding materials.

Keywords: Composites, Silicone rubber, Shielding effectiveness

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DOI: https://dx.doi.org/10.5281/zenodo.1170794

Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials

Temperature dependencies of dielectric properties in $Na_{1-x}K_xTaO_3$ system

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Pellet samples of mixed sodium-potassium tantalate ($Na_{1-x}K_xTaO_3$), for compositions x = 0, 0.2 and 0.5 were prepared by solid-state reaction method. The calcined mixture was pressed at 0.02 MPa and sintered in a closed furnace to form 6 mm diameter pellets. Temperature variation of dielectric constant and loss tangent of the prepared samples has been studied in the frequency range from 10 KHz to 1 MHz. Dielectric anomalies have been observed near the transition temperatures of the samples. Dielectric constant and loss tangent peak heights were observed decreasing with increasing frequency, for all the compositions, which show relaxational behavior of the material.

Keywords: Ferroelectrics, perovskite, dielectric constant, loss tangent, sintering.

DOI: https://dx.doi.org/10.5281/zenodo.1168759

Phase Coexistence and Structure of Coexisting phase in a New Perovskite Solid Solution $xBa(Cu_{1/3}Nb_{2/3})O_3–(1-x)PbTiO_3$

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Abstract

The motivation to replace the commercial high performance piezoelectric lead zirconate titanate (PZT) with a nontoxic substitute has led to a great surge in research interest in lead-free piezoelectric in the last decade [1]. In this context, it may be worth mentioning that a very large piezoelectric response is obtained when relaxor ferroelectrics $Pb(Mg_{1/3}Nb_{2/3})O_3$ and $Pb(Zn_{1/3}Nb_{2/3})O_3$ are alloyed with ferroelectric $PbTiO_3$. In this work, a new solid solution $xBa(Cu_{1/3}Nb_{2/3})O_3–(1-x)PbTiO_3$ (x=0.30, 0.35, 0.38, 0.40, 0.42 and 0.45) ferroelectric ceramics were prepared using conventional solid state route and its formation was ascertained by X-ray diffraction method. Rietveld refined X-ray diffraction data of all the ceramics suggested the crystal structure change from tetragonal (P4mm) to cubic (Pm3m) symmetry with the increase in $Ba(Cu_{1/3}Nb_{2/3})O_3$ concentration (x). Average grain size is observed in the range of 1.5~2.5μm for samples sintered at 1050°C for 2 hour. Variation of dielectric constant and dielectric loss with temperature show diffuse ferroelectric characteristics.

“Keywords: X-ray diffraction; Lead-free Piezoelectric; Dielectric; SEM”.

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DOI: https://dx.doi.org/10.5281/zenodo.1170796

Studies on effect of B-Site substitution on LSCF perovskite ceramics for membrane applications

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Abstract

Cobalt based perovskite oxides are advantageous for membranes applications since cobalt is beneficial for the activation of the oxygen molecules. However the reduction behavior of cobalt at high temperature leads to a structure transition which in turn results in decrease of oxygen ion transport through the membranes [1, 2]. The present work focuses to study the effect of B-Site substitutions on the perovskite system $(La,Sr)(Fe,B)O_{3-\delta}$ (B = Zn, Co, Al) and to develop the cobalt free perovskite for membrane applications. The perovskite MIEC oxide has been prepared using solution combustion technique. It is observed that the structural parameters like lattice parameter, tolerance factor, saddle point radius, average metal oxygen bond energy, free lattice volume were increased with decrease in the ionic radius of B-site cation. The temperature dependent electrical conduction behavior of the samples showed small polaron hopping mechanism at low temperature and metallic conductivity behavior at high temperature. It has been observed that the time constant for the electrical conductivity relaxation is more in case of Al substituted samples which might be due to the presence of high ionic conductivity compared to the Zn substituted samples. Further this electrical conduction study is correlated with the microstructure of the samples.

Keywords: LSCF, electrical properties, microstructure.

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DOI: https://dx.doi.org/10.5281/zenodo.1170798

Orbital Order-Disorder Transition in Doped Perovskite Manganites: Influence of Intrinsic Octahedral-Site Distortion

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Abstract

The orbital order-disorder transition temperature (T_{OO}) versus tolerance factor (t) plot switches from monotonic to non-monotonic beyond a doping level (x) ~10 atom% in a family of $R_{1-x}A_xMnO_3$ systems (R = La, Pr, Nd; A = Ca, Sr; x = 0.0-0.2). T_{OO} reaches maximum at a 'doping-dependent' critical tolerance factor $t_C(x)$ at which the orthorhombic distortion (D) also maximizes. Such an observation reflects influence of charge carriers on both 'intrinsic' octahedral-site distortion itself and its bias on the orbital order in doped perovskite manganites and, thus, deviation from what has been observed in undoped $RMnO_3$, $RTiO_3$, and RVO_3 systems where maximization of T_{OO} and D takes place at a universal tolerance factor or R-site ion size [1-3].

Manganite, Orbital order, Strongly correlated electron system, Tolerance factor

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DOI: https://dx.doi.org/10.5281/zenodo.1170800

An azide-functionalized Al(III)-based metal-organic framework for the fast, selective and highly sensitive detection of exogenous and endogenous H_2S

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Abstract

MOFs, which are a new class of crystalline porous compounds, possess versatile application potentials ranging fromgas storage/separation, chemical sensing and heterogeneous catalysis to biomedical imaging and drug delivery [1]. A new, azide-functionalized Al(III)-based metal-organic framework (MOF) denoted as CAU-10-N_3 (**1**, CAU = Christian-Albrechts-University) and consisting of 5-azido-isophthalic acid (H_2IPA-N_3) ligand was employed as a reaction-based fluorescent turn-on probe for the detection of H_2S. The activated compound (**1′**) showed fast, selective and highly sensitive sensing properties for extracellular H_2S in HEPES buffer. The limit of detection of **1′** for H_2S is 2.65 μM, which is lower than the earlier reports on MOFs for H_2S sensing. The material displayed short response time (420 s) and significant increase (20-fold after 1 minof addition of Na_2S) in the fluorescence intensity towards H_2S. Macrophage cells loaded with probe **1′** exhibited blue fluorescence with a response time of 15 min after Na_2S addition, indicating the suitability of the probe for intracellular H_2S detection.

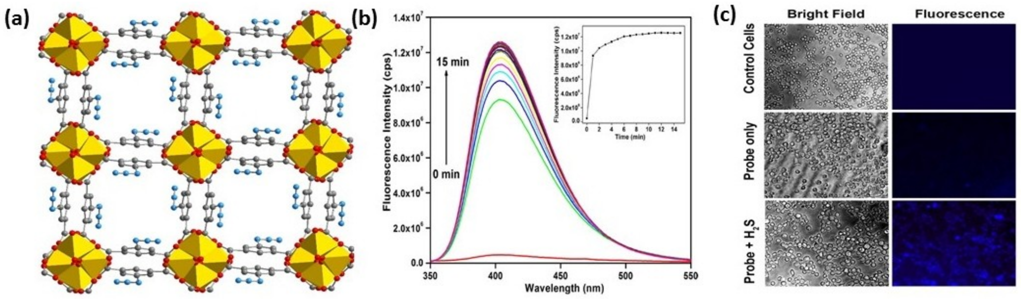

Fig. 1.(a) Structure ofthe CAU-10-N_3MOF.(b) Fluorescence turn-on response of the MOF suspension in HEPES buffer(10 mM, pH = 7.4) towards addition of Na_2S. (c) Ability of the MOF to detect H_2S in macrophage J774A.1 cells.

Keywords: metal-organic framework, azide-functionalization, fluorogenic probe, H_2S sensing, cell imaging.

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DOI: https://dx.doi.org/10.5281/zenodo.1170804

Post-synthetic modification of a metal-organic framework fordualnaked-eye fluorogenic detectionin aqueous medium

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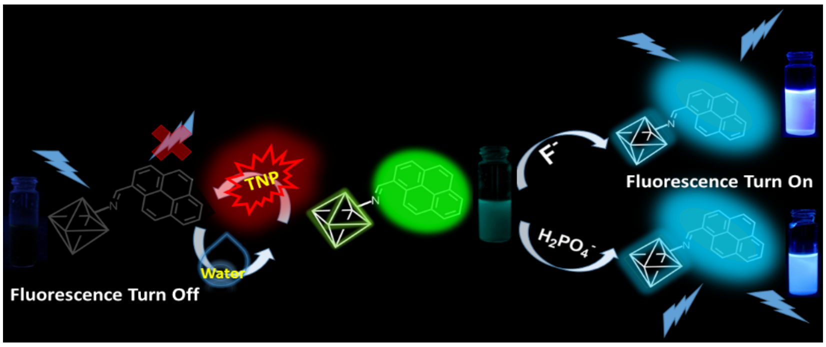
Abstract

As a new generation of crystalline porous materials, metal-organic frameworks (MOFs) have received tremendous attention in recent years not only owing to their intriguing structures but also for their potential applications in gas storage, heterogeneous catalysis, drug delivery and fluorescent sensors.

The metal-organic framework (MOF) called UiO-66-NH_2 (**1**; UiO = University of Oslo) was post-synthetically modified by condensation with 1-pyrenecarboxaldehyde. The pyrene-tagged MOF (**1'**) exhibited ~3-fold enhancement in fluorescence intensity over the un-functionalized one with a new emission peak at 470 nm due to the formation pyrene excimer within the framework. **1'** showed fast response time, excellent selectivity and sensitivity for sensing of biologically active anions like F^- and $H_2PO_4^-$ in pure aqueous medium via fluorescence ‘turn-on’ mechanism. **1'** also displayed rapid, selective and sensitive detection of 2,4,6-trinitrophenol (TNP) in aqueous medium via fluorescence ‘turn-off’ mechanism. The excellent detection performance of **1'** in aqueous medium makes it a promising dual sensor material for real-field applications.

Keywords: Metal-organic framework, Post-synthetic modification, Anion sensing, Nitroaromatics sensing.



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DOI: https://dx.doi.org/10.5281/zenodo.1170810

Rietveld structural analysis of new Bi-based piezoceramics with morphotropic phase boundary

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Recently several Bi-based piezoelectric solid solutions with reduced Pb-concentration such as (1-x)$Bi(Mg_{1/2}Zr_{1/2})O_3$-x$PbTiO_3$ (1), (1-x)$Bi(Ni_{1/2}Ti_{1/2})O_3$-x$PbTiO_3$ (2), (1-x)$Bi(Mg_{1/2}Ti_{1/2})O_3$-x$PbTiO_3$ (3) etc. have been investigated to develop better alternative of widely used $PbZr_xTi_{1-x}O_3$ due to growing concern about toxicity of lead. Further, many applications under non ambient conditions, require high Curie Temperature (T_C) such as actuators and transducers for automotive industries, space technology etc. for which Bi-based morphotropic phase boundary [MPB] ceramics have shown considerable promise. The structural investigation of these solid solutions by Rietveld method reveals coexistence of phases in the MPB region and appearance of new low symmetry monoclinic phase. In this seminar, I will present the results of Rietveld structural investigations on the structure of the coexisting phases and phase transitions in these piezoelectric ceramic solid solutions. I will also discuss the resutls of structural investigations on electric field poled (1-x)$Bi(Mg_{1/2}Ti_{1/2})O_3$-x$PbTiO_3$ and (1-x)$Bi(Mg_{1/2}Zr_{1/2})O_3$-x$PbTiO_3$ piezoceramics across morphotropic phase boundary that reveals significant modifications in crystal structure. The pseudocubic monoclinic phase outside the phase coexistence region in (1-x)$Bi(Mg_{1/2}Ti_{1/2})O_3$-x$PbTiO_3$ undergoes isostructural phase transformation to long range monoclinic phase with significantly larger lattice parameters than that in the unpoled state (4). In contrast the pseudocubic composition of (1-x)$Bi(Mg_{1/2}Zr_{1/2})O_3$-x$PbTiO_3$ transforms to tetragonal phase after electric field poling (5).

Keywords: Bi-based Piezoelectric MPB Ceramics, Rietveld Refinement, Electric Field Induced Phase Transition.

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DOI: https://dx.doi.org/10.5281/zenodo.1170816

Large negative magnetoresistance and thermal properties of $Ni_{50-x}Mn_{37+x}Sn_{13}$(x = 0, 1, 2, 3) Heusler alloys

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Electrical resistivity and magnetoresistance for $Ni_{50-x}Mn_{37+x}Sn_{13}$ (x = 0, 1, 2, 3) have been investigated. In $Ni_{47}Mn_{40}Sn_{13}$, a negative magnetoresistance of 56 % is attained at a field strength of 5T. The drastic change in resistivity upon martensitic transformation is observed for all alloys. The magnetoresistnace increases with Mn concentration. The increase in magnetoresistance is ascribed by the super zone boundary gaps. We also investigated thermopower S and thermal conductivity κ for $Ni_{50-x}Mn_{37+x}Sn_{13}$ (x = 0, 3) alloys in order to further characterize the heat transport. The S shows an overall negative sign signifying the electron type charge carriers dominate in this compound. The negative S decreases with increase in Mn concentration.

DOI: https://dx.doi.org/10.5281/zenodo.1170824

STRUCTURAL AND VIBRATIONAL STUDIES ON CO-CRYSTAL: 5-FLUOROURACIL 4-AMINO BENZOIC ACID

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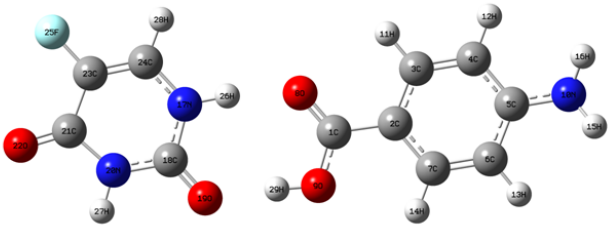
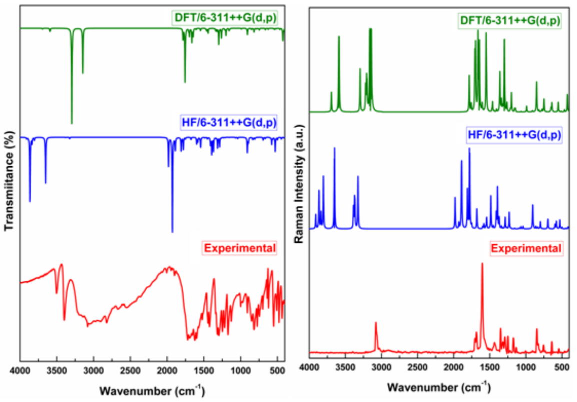
Abstract

The fluorine based compounds received the attention of many pharmaceutical scientist around the world for the past few decades. Because, the presence of fluorine as a functional element in the pharma drug highly alter its physicochemical and biological properties. 5-Fluorouracil is one of the fluorine-based derivatives and a well-known anticancer drug. It was first prepared in 1957 and used in the treatment of solid tumors, such as colorectal, breast, gastrointestinal and ovarian cancers.





The geometries obtained from the single crystal XRD of the cocrystal, namely 5-fluorouracil 4- amino benzoic acid (5FU4AMBZ) was optimized theoretically by the 6-311++G(d,p) method on a Intel Core i5/ 3.20 GHz computer using Gaussian 09W program package. The optimized C–F bond length is 1.317 and 1.341 Å in HF and DFT/B3LYP methods respectively. The corresponding bond length is good agreement with the single crystal XRD studies. The C–N bond distance varies from 1.354 Å to 1.389 Å and 1.370 Å to1.411 Å in HF and DFT methods for the present compound. The solid state values are obtained to 1.355 (1), 1.369 (1), 1.381 (1) and 1.387 (1) Å. The present molecule has different functional groups like –N–H, –C–H, –C–C, –C=O and –OH. Normally, the N–H stretching vibration of the all the co-crystals are appeared in the range of 3000–3230 cm^{-1}. The medium intensity peak observed at 3499 cm^{-1} in IR spectra is attributed to the N–H stretching vibration for the 5FU4AMBZ molecule.

DOI: https://dx.doi.org/10.5281/zenodo.1170826

Approach to synthesis and improving the solubility of a bronchodilator drug (Theophylline) by its salts and cocrystals.

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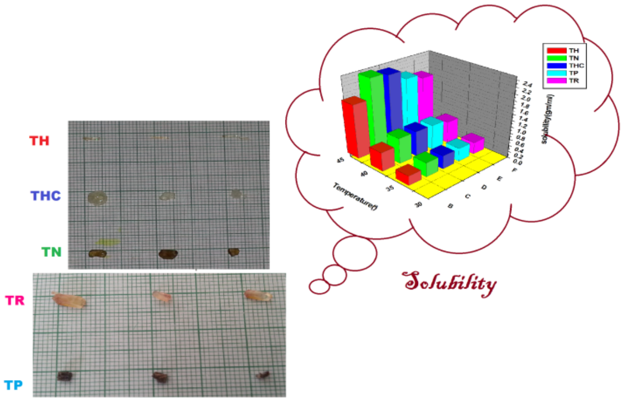
**E-mail: crystallographer@rediffmail.com*

Theophylline is considered as one of the most important pharmacologic compounds. For a long period of times, synthetic drugs of theophylline have been used in the treatment of more severe diseases resulting from disorder in the physiological functions of pulmonary system, such as asthma and COPD. The cocrystal formation of theophylline with dicarboxylic acids such as oxalic acid, glutaric acid, maleic acid and dipicolinic acid, pyrazole dicarboxylic acid have been the leading task of the researcher. Also, the application of crystal engineering expands its cocrystal field to multi-drug resistance, enhancing drug action thereby reducing the side effects of the drugs. The crystal structure of THC monohydrate was an earlier reported one and compared with the parent (TH). The crystal and molecular structures of new Theophyllinium Nitrate (TN), and Theophyllinium Chloride (THC) salts were analyzed by single crystal X-ray diffraction method. Also a new Theophylline pyrogallol (TP) and a redeterrmination work of Theophylline resorcinol (TR) were studied by single crystal X-ray diffraction. The aim of present investigation is to synthesis and increase the solubility of the drug thereby improving the biological and chemical entity.



The solubility test has been carried out for both the salts and cocrystals to enhance the drug solubility and the therapeutic effectiveness of the drug. Also, the compounds were examined for its antibacterial activity and found to exhibit notable activity in TN against *Pseudomonas aeruginosa*. Hence the new compound TN is a good candidate for the antimicrobial agent apart from its inherent Bronchodilator drug property.

DOI: https://dx.doi.org/10.5281/zenodo.1170830

Synthesis of New polycyclic Hetero-Aromatic Hydrocarbons and their photophysical studies

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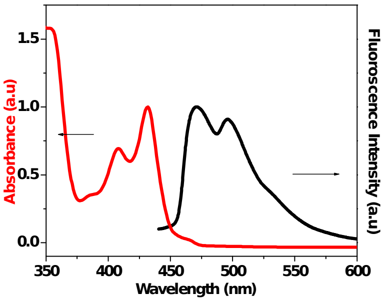
Synthesis of polycyclic hetero-aromatic hydrocarbons (PHAHs) and elucidate their solid state structures in crystals. The synthesis fully here is simple and provides easy access to this important class of materials.[1]One of the most frequently used methodologies for this purpose is the aromatic framework of PHAHs to improve their physicochemical properties and enhance the carrier transport of the system for applications as organic field-effect transistors.[2]We have designed and synthesized a new family of PHAHs containing a tetracene core which can be synthesized from aldehydes using a various – steps such assequence of Mcmurry coupling, Diels – Alder reaction and scholl reaction oxidative aromatization under mild conditions to give final product.



Keywords: Polycyclic hetero-aromatic hydrocarbons, Organic Field-effect Transistors, and Tetracene

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DOI: https://dx.doi.org/10.5281/zenodo.1168764

High Performance Au-decorated ZnO 2D-Nanosheetsfor NO_2 Gas Sensing Applications

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Abstract:

Nitrogen dioxide (NO_2) is a highly toxic environmental pollutant,which is mainly produced by emissions from power plants, combustion engines and automobilesand can cause serious health hazards. Therefore, detection of such harmful pollutants is a serious demand for environmental monitoring. Herein, we report the synthesis, characterization and evaluation of NO_2 gas sensor properties of ZnO@Au heterojunction 2D nanosheets to develop a reliable sensor that can effectively detect NO_2at trace-level concentrations.Two-dimensional nanostructures are highly attractive for fabricating nanodevices due to their high surface-to-volume ratio and compatibility with device design. Structural and morphological analyses havebeen carried out usingXRD,HR-TEM,UV-Visible and fluorescence spectrum. The temperature dependent *I-V*characteristic of 2D ZnO-Au nanosheets was used to explore the electron transport properties of the nanosheets. The gas sensing propertiesof the ZnO nanosheets wereanalyzed whichexhibited high sensitivity for detecting NO_2 at lower working temperature.The catalytic behaviourof Au found to enhance the sensor response towards NO_2.

Keywords:*ZnO Nanosheets, heterojunctions,NO_2gas sensor, Au-catalytic behaviour.*

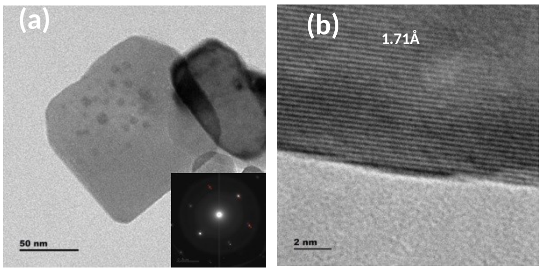

Figure: (a) TEM image of ZnO@Au nanosheets,inset shows corresponding SAED pattern, (b) HR-TEM image of ZnO nanosheets

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DOI: https://dx.doi.org/10.5281/zenodo.1170677

Magnetoelectric coupling in antiferromagnet $Co_4Ta_2O_9$

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Abstract

We study themagnetoelectric(ME) coupling in spin-flopdriven antiferromagnet $Co_4Ta_2O_9$.The dielectric constant and pyroelectric current show features associated with ferroelectric transitions at the antiferromagnetic transition temperature (T_N =20 K). The effect of magnetic field is to enhance the features almost linearly up to the maximum measured field (6 T) with a saturation polarization value of 52μC/m^2.

Keywords:Magnetoelectric materials, Electric polarization, Magnetization.

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DOI: https://dx.doi.org/10.5281/zenodo.1170696

Effect of reaction time on the synthesis of InAs nanowire via solvothermal route

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Abstract

Wehave synthesized InAs nanowires (NWs) by using solvothermal methodswith the increase in reaction time from 30 min. to 2 hour. Structural analysis has been done by using FESEM (Field Emission Scanning Electron Microscopy). The nanowire has diameter in the range from 40-60 nm, whereas length up to 10 micro metre. Raman spectra was obtained in the spectrum range 170-280 cm^{-1} shows the redshift in the LO (Longitudinal Optical) and TO (Transverse Optical) mode, whereas blueshift in the SO (Surface Optical) phonon mode. Broadening in the TO and SO mode for InAs NWs with the increase in the reaction time t = 30 min. to 1 and 2 Hour. The quantum confinement effect in NWs results downward frequency shift and broadening of TO and SO mode due to the relaxation of the q = 0 selection rule in the Raman scattering.

DOI: https://dx.doi.org/10.5281/zenodo.1170848

ZnS based Core shell Quantum Dots for next generation Bio-imaging

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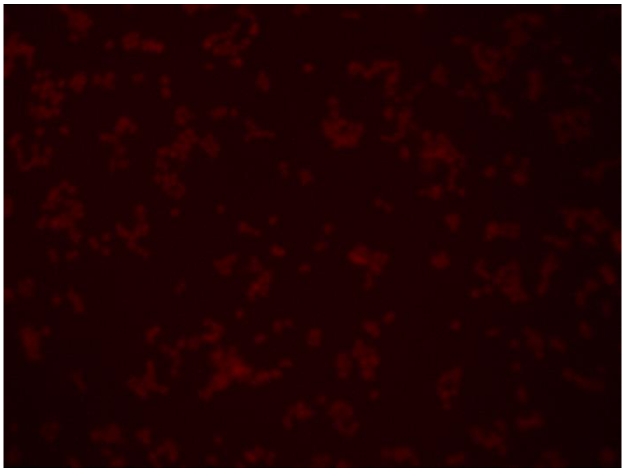
Abstract

ZnS is a wide band gap semiconductor and it shows remarkable properties that can be exploited for versatile applications including transistors, LEDs, biology and medicine etc. ZnS based core shell nanoparticles is prepared by co-precipitation technique with edible dye as the shell. The absorption and PL measurements shows their absorption maximum at 499 nm. The nano particles are incubated in Hela cells and monitored cellular uptake and fluorescence.



Fluorescence image of Hela Cell

Keywords: ZnS Nanoparticles, Surface Plasmon Resonance, Hela

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DOI: https://dx.doi.org/10.5281/zenodo.1170717

Influence of oxygen vacancies on structural and electrical properties ferromagnetism imposed ferroelectric material

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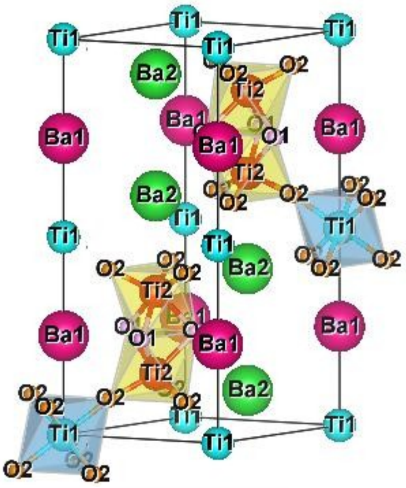
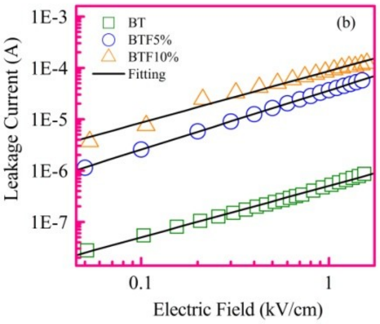
Abstract

$BaTi_{1-x}Fe_xO_{3-\delta}$ ceramics have been prepared by solid state reaction route. Effect of oxygen vacancies on structural and electrical properties of Fe-substituted $BaTiO_3$ is investigated. From Rietveld refinement, tetragonal (P4mm) and orthorhombic (Amm2) phases occur in pure $BaTiO_3$ [1] while tetragonal (P4mm) and hexagonal ($P6_3$/mmc) in Fe-substituted $BaTiO_3$. Cell parameters, volume fraction and oxygen vacancies are also obtained from Rietveld refinement. Hexagonal unitcell was drawn using VESTA. Ti1(2a) and Ti2(4f) are located in the center of corner-shared TiO_6 octahedra and face-shared Ti_2O_9 dimer respectively. Leakage current is increased almost 2 orders of magnitude in Fe-substituted $BaTiO_3$ than pure $BaTiO_3$ which is due creation of oxygen vacancies for charge compensation. Calculated δ values are 0.188 and 0.282. Present work revels that oxygen vacancies play an important role in structural and electrical properties of ferromagnetism imposed in a ferroelectric material.





Keywords: $BaTiO_3$, Rietveld refinement, oxygen vacancy, multifunctional material.

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DOI: https://dx.doi.org/10.5281/zenodo.1170849

Properties of TiO_2 doped SnO_2 thin films deposited using jet nebulizer spray pyrolysis technique for sensor analysis

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[2] Research Scholar, Bharathiar University, Coimbatore

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Abstract

Oxides, metallic materials and functional layers in commercial electronics applications and sensor devicesare deposited using the jet nebulizer technique. The coatings of intrinsic and extrinsic varieties of SnO_2 are employed on a large scale of optoelectronic devices. Extra mural studies were also extended towards the various factors of the thin film, the effect of substrate temperature, electrical conductivity, mobility, carrier concentration as well as feasibility of developing high quality conducting oxide thin films. SnO_2-TiO_2 NPs are nanometer-sized, bright, photo stable, bio-specific, non-toxic that would be used to remove the heavy metal analysis. Since TiO_2 and SnO_2 are insoluble in water, less expensive and higher photocatalytic efficiency semiconductors were selected as the photocatalysts and these find applications in the removal of heavy metals from contaminated water sources in addition to the electronic uses.The development of an aqueous and environmental friendlier synthesis route of jet nebulizer techniques for TiO_2: SnO_2 thin films and the characterization of the deposited films, a study on the impact of substrate temperature on the structural, optical, electrical, and morphological properties of TiO_2: SnO_2 films deposited by the JNS pyrolysis technique, the results for the optimization of the temperature for the formation of crystalline TiO_2: SnO_2 films with aSn-doping concentration,an application of the developed thin films for the effective removal of toxic heavy metals such as lead and mercury were carried out.

Keywords: JNS pyrolysis technique, TiO_2-SnO_2 thin films, Photocatalysts

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DOI: https://dx.doi.org/10.5281/zenodo.1170850

Magnetoresistance Properties of $BaTi_{1-x-y}Fe_xNb_yO_3$ Ceramics

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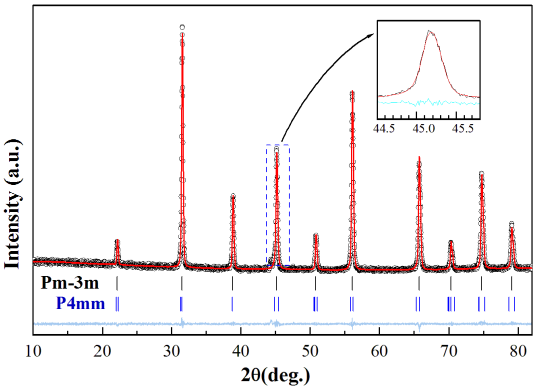
Abstract:

Magnetoresistanceand magnetodielectricpermittivity under an applied magnetic field has been investigated to develop a new multifunctional device using multiferroic $Ba(Ti_{1-x-y}Fe_xNb_y)O_3$(BFNT) material at room temperature. Samples with x,y=0, 0.025, 0.05 and 0.075 were prepared using solid-state reaction method. BFNT has a mixture of tetragonal (*P4mm*) and cubic (*Pm-3m*) phases. The cubic phase fractionis increased with *x*, y-mole fraction which is revealed from Rietveld refinement. Magnetoresistance &magnetodielectric studies at different frequencies and P-E, M-H hysteresis loops are also investigated. Large negative magnetoresistance (MR) andmagnetodielectric constant (MDC)are observed with the addition of Fe and Nb. Intrinsic and extrinsic contributions play a significant role in the MR and MDCand this has been explained by Maxwell Wagner effect and magnetostriction [1].



Keyword: Ferroelectric properties, magnetic properties, Magnetodielectric and magnetoresistance properties.

Reference

1. Dhiren K. et al J. Appl Phys**114**, 234106 (2013)

DOI: https://dx.doi.org/10.5281/zenodo.1170854

Synthesis and Magnetic Properties of Magnesium Ferrite Nanoparticles

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Magnesium ferritenanoparticleswere synthesized using co-precipitation and sol-gel methods. The nanoparticle samples were annealed at different temperatures in air for 4 hours. All the samples were single phase except the sol-gel sample annealed at 700˚C which showed presence of α-Fe_2O_3. The grain size was found to be 28-33 and 15-50nm for these nanoparticle samples prepared by co-precipitation and sol-gel methods respectively. The magnetization value increased with the increase in annealing temperature in the samples prepared by co-precipitation method where as the samples prepared by sol-gel method did not show any systematic variation. The highest magnetization valuesof 34 and 24 emu/g were observed at 300K for the samplesannealed at 900˚C prepared by co-precipitation and sol-gel methods respectively. The blocking temperature was found to be increased with the increase in grain size in the zero field cooled magnetic measurement. The observed magnetic behavior can be explained on the basis of different synthesis methods and grain growth in these samples.

Keywords: Ferrite, nanoparticles, Magnetization,Coercivity

DOI: https://dx.doi.org/10.5281/10.5281/zenodo.1170774

Highly active multimetallic nano alloys embedded in conducting polymer: Implementation in fuel cells and photocatalysis

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Abstract

Conducting polymer nanostructures has been recognized as photocatlysts, a promising breakthrough in photocatalysis and other energy conversion application, such as fuel cell and battery in the near future (1, 2).A facile method has been developed for the synthesis of Pd, and Pt nanoparticles (NPs) based multimetallicnanoalloys incorporated on polypyrrole (Ppy) nanofibers by colloidal radiolytic technique (3, 4). Metal nanoparticle is uniformly deposited on polypyrrole nanofibers, showing a significantly high eletrocatalytic activity and durability compared with the Pd/C catalyst for electroxidationof methanol or ethanol.The ultrasmall $Pd_{30}Pt_{29}Au_{41}$/Ppy nanohybrids (~8 nm) exhibit an excellent electrocatalytic activity which is ~5.5 times higher than monometallic counter parts (12 A per mg Pd, 5 times higher activity compared to Pd/C catalyst).An efficient light harvesting hybrid nanostructures based on Poly(3,4-ethylenedioxythiophene) (PEDOT) nanofibers and gold nanoparticles (Au NPs) was prepared successfully *via* an one pot colloidal synthetic route. The plasmonic Au NPs (~6 nm) are synergistically integrated on the conductive polymer nanofibers as evident from microscopic techniques. The Au/Ppy nanohybrids (NHs) demonstrate superior photocatalytic activity for organic pollutant degradation under visible light irradiation which is ~5.6 times higher than bare polymer.

Keywords: Conducting polymer nanostructures, Nanohybrids, Metal nanoparticles, Visible light active photocatalyst, H_2 generation

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DOI: https://dx.doi.org/10.5281/10.5281/zenodo.1170780

Lattice strain induced structural phase evolution in BNT-BNZ solid solution

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Abstract

The polycrystalline lead free (1-x) $Bi_{0.5}Na_{0.5}TiO_3$-(x)$Bi_{0.5}Na_{0.5}ZrO_3$ [BNT-BZT]with x= 0.10-0.50 based solid solutions have been prepared by the high temperature solid state ceramic method. X-ray diffraction analysis confirms the formation of single phase stable perovskite compound. Structural phase transition from rhombohedral (*R3c*) to orthorhombic (*Pnma*) crystal symmetry with the increase of mole fraction of Zr^{4+} in BNT has been observed from the Rietveld refinement of XRD patterns. The structural evolution between *R3c* and *Pnma* crystal symmetries in the present solid solutions can bewell explainedby assuming thelattice strainin the crystal structure. It is basically due to the mismatch of ionic radii between titanium (Ti^{4+}~0.60pm) and zirconium (Zr^{4+}~0.72pm).Also, variation of the crystal symmetries of the solid solutions has been correlated with Goldschmidt tolerance factor (t). The microstructure of the solid solutions is analyzed by the field emission scanning electron microscopy (FE-SEM), which confirmed the formation of dense ceramic with non-uniform grain size. Room temperature Raman spectra of all the solid solutions have been investigated to confirm the structural phase transition by observing the variation in different mode of phonon vibrations. The room temperature dielectric permittivity of the solid solutions has been measured in the frequency range from 100 Hz to 1MHz. It is observed that the composition with x =0.35 exhibits maximum dielectric constant, which is identified as morphotropic phase boundary composition.

Keywords: Dielectric, Rietveld, XRD, Crystal structure, Lattice strain

DOI: https://dx.doi.org/10.5281/10.5281/zenodo.1170786

Guest Molecules in the Cages of Clathrate Hydrates: A Theoretical Study to Evaluate the Storage Capacity

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Abstract: Density functional theory (DFT) based studies are carried out to understanding structure, stability and reactivity of clathrate hydrates with or without hydrogen encapsulation. All geometries of clathrate hydrate were fully optimized using B3LYP/6-31G(d)//M06-2X/6-31G(d)//B97D/6-31G(d) level of theory. We systematically explore the gas capability of five standard water cavities (5^{12}, $4^{3}5^{6}6^{3}$, $5^{12}6^{2}$, 5^{12} 6^{4} and $5^{12}6^{8}$) in clathrate hydrate. We have select for maximum cage occupancy of the five different cages (5^{12}, $4^{3}5^{6}6^{3}$, $5^{12}6^{2}$, 5^{12} 6^{4} and $5^{12}6^{8}$) is one, two, three, four and five guest molecules in every cages. We used as a guest molecules Ar, CH_4, CO_2, H_2, H_2S, Kr, N_2, O_2 and Xe respectively. The maximum and optimum cage occupancy for all five considered cages as a guest molecule in the clathrate hydrate one, one, two, three, and four for CH_4, one, one, two, three, and four for CO_2, one, one, two, four and five for H_2, one, one, two, three, and four for O_2, one for all Xe, one, one, two, three, and four for Ar, one, one, two, three, and four for H_2S and one, one, two, three, and four for Kr. The efficacy of trapping of hydrogen molecules inside the cages of clathrate hydrates depends upon the cavity sizes and shapes of the clathrate hydrates. The efficacy of trapping of hydrogen molecules inside the cages of clathrate hydrates depends upon the cavity sizes and shapes of the clathrate hydrates.

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Keywords: Gas Hydrates; Clathrate Hydrates; Density Functional Theory

DOI: https://dx.doi.org/10.5281/zenodo.1170792

Quantitative HRTEM Analysis of Strain Assessment along the Defect Cores in Cryo-rolled CP Ti

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Microscopic and functional manifestation of strains in materials originates from local imperfections in the atomic scale, which essentially depicts shifting of the atom coordinates from their mean equilibrium positions. Hence an estimate of the atomic shift provides the much needed clue to analyze the induced strain in the materials because of defect formation, alloying addition or through metallic deformation. In the present work, a quantitative estimation of strain has been carried out along the defect cores of severely cryo rolled CP Ti from the aberration corrected atomic resolution TEM micrographs.

Image aberration corrected phase contrast micrographs, which are already well analyzed in terms of structural information, are subjected to the investigation of Geometrical Phase Analysis (GPA) to generate the strain map. The map has been normalized with respect to the minimum strain region. Relative variations of strain across the defect cores have been generated. A typical micrograph is shown in fig 1(a). However in the atomic resolution images several linear contrasts can be observed which are postulated to be originated from the accumulation of the localized strain during rolling. Multislice image simulation in a systematic manner has been carried out (fig 1b) to eliminate the effects of defocus, thickness and the alloying elements in the generation of these linear contrasts. Quantitative electron microscopy analyses using the GPA methods are employed to confirm the generation of these linear contrasts due to the localized strains as shown in fig 1(c).

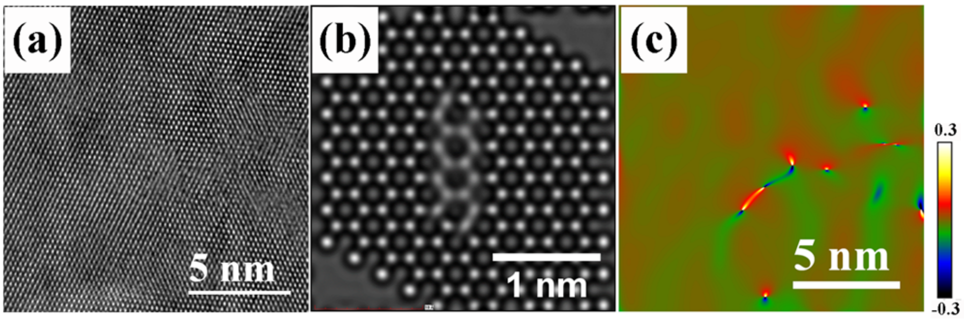

Fig. 1(a-c) Image corrected HRTEM micrograph, corresponding simulated image and the localized strain map from a severely deformed CP Ti specimen.

DOI: https://dx.doi.org/10.5281/10.5281/zenodo.1170802

Synthesis and Characterization of Vanadium Pentoxide for Methane gas sensing

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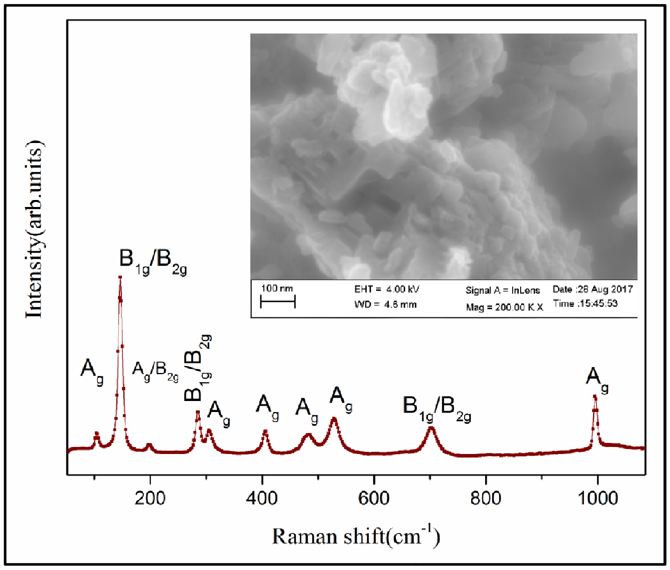
Abstract

Vanadium pentoxide (V_2O_5) has drawn significant interest in the past few decades due to its various applications such as in gas sensors, thermochromic devices, optical switching devices etc. A near room temperature gas sensor is required to detect methane from coal mines, power plants and marshy areas. In the present study orthorhombic α-V_2O_5 has been synthesized by low cost and simple hydrothermal method using aqueous solution of ammonium metavanadate. The crystal structure has been identified by XRD. The presence of peaks at 146 $cm^{-1}$and 996 cm^{-1} in the Raman spectrum confirms the signature of V_2O_5. FESEM images revealed the size of nanoparticles to be in the range of 30-50nm. The nanostructures showed response towards 500ppm methane gas at 100°C operating temperature.



Keywords: Vanadium pentoxide, Hydrothermal method, Methane sensing

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DOI: https://dx.doi.org/10.5281/zenodo.1170818

Ultrasonic velocity studies on $Ni_xCo_{1-x}Fe_2O_4$ nanoferrofluid prepared by co-precipitation method

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Abstract

Nanoferrofluids of $Ni_xCo_{1-x}Fe_2O_4$ were prepared by chemical co- precipitation method by varying the value of *x* (0.1, 0.3, and 0.5M). The structural characterization done by X- ray diffraction (XRD) confirms the formation of spinel ferrite structure. The crystallite size of the samples calculated using Scherrer formula from the full width half maximum of (3 1 1) plane are in the range of 33 – 42 nm. The crystallite size of the sample increases with increase in nickel content. The surface morphological investigation was done by scanning electron microscopy (SEM) technique. The ultrasonic velocity of nickel doped Cobalt nanoferrofluids was measured by varying the temperature in the range of 30-70 ^{o}C. The ultrasonic velocities of magnetic nanoferrofluids decrease with increase in nickel concentration. The higher value of velocity of nanoferrofluid than that of the carrier liquid in the absence of magnetic field shows the influence of dispersed particles on the velocity of ultrasonic propagation.

Keywords: Nanoferrofluids, Ultrasonic velocity, Crystallite Size, Co- precipitation method

DOI: https://dx.doi.org/10.5281/zenodo.1170832

Synthesis and characterization of Dye sensitized solar cells using natural dye extracted from blue pea flowers

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Abstract

Nanostructured TiO_2 thin films were prepared by spin coating method on fluorine - doped tin oxide (FTO) plate at 6000rpm. The structural characterization done by X-ray diffraction (XRD) reveals the formation of rutile phases of TiO_2. The crystallite size of the sample calculated by Scherrer formula from the full width half maximum of (1 1 0) plane is 21 nm. The natural dye (anthocyanin) was extracted from Blue pea flower by using ethanol and their pH values (3.2, 3.4 and 3.6) were varied by adding 0.1M of HCl. The photoanode required for DSSCs was prepared by sensitizing TiO_2 thin films with these dye solutions. The band gap of the samples calculated from Ultraviolet visible (UV –Vis) and Photoluminescence (PL) techniques are in the range of 2.5 to 2.7 eV. The DSSCs prepared were using these photoanodes were characterized by I-V measurements using Keithely source meter. The DSSC prepared from the dye having pH = 3.2 has shown maximum conversion efficiency of 0.026 %.

Keywords: Natural dyes, Anthocyanin, Photoluminescence, DSSC.

DOI: https://dx.doi.org/10.5281/zenodo.1170838

A study on the effect of dye sensitizers on nanostructured GaAs/PS based DSSCs

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Abstract

Nanostructured porous silicon (PS) sample were prepared at a current density of 30 mA/cm^2 for etching periods 60 minute. The Gallium Arsenide (GaAs) is used as a nanofillers to fill the PS samples. The XRD patterns reveal the formation of PS and GaAs on PS. Then the photoanodes were prepared by sensitizing the surfaces of these PS+GaAs samples with various dyes such as chloroaluminium phthalocyanine (ClAlPc), N7 and Eosin – Y (EY). The bandgap of the samples foundd from Photoluminescence (PL) spectrum are in the range of 1.9 – 2.0 eV. The photocurrent and photovoltage of the cells weres measured using Keithely source meter. The maximum conversion efficiency of 2.8% is observed and results are discussed.

Keywords: Porous Silicon**,** GaAs, Photoluminescence, DSSC.

DOI: https://dx.doi.org/10.5281/zenodo.1170840

A Study on the Effect of pH Values on Magneto-Optic Properties of Fe_3O_4 Nanoferrofluids

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Abstract

Fe_3O_4 nanoparticles have been synthesized at different pH values of co-precipitator (NaOH) using co-precipitation method with oleic acid as surfactant. Structural characterization was done using X-ray diffraction (XRD) technique and the crystallite sizes of the samples were calculated by Scherrer approximation from the full width half maximum value of (311) plane. The particle sizes are in the range of 6.48nm, 7.18nm and 7.66nm. Surface morphology and the chemical composition of the samples were investigated using Scanning electron microscope (SEM) with EDAX analysis. Magnetic parameters of the sample such as Saturation magnetization (M_s), Remanence (M_r) and Coercivity (H_c) were measured using vibrating sample magnetometer (VSM) at room temperature. Verdet constant of the samples were calculated from Faraday rotation for various magnetic fields and it varies from 5.02×10^{-4} deg./G cm to 8.04×10^{-4} deg./G cm.

Keywords: Co-precipitation, Saturation Magnetization, Remanence, Coercivity, Faraday rotation, Verdet constant.

DOI: https://dx.doi.org/10.5281/zenodo.1170842

Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials

Thermally driven resistive switching in solution-processable thin films of coordination polymers

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Abstract

Metal−organic coordination polymers (CPs) downsized to thin films with controllable electrical conductivity are promising for electronic device applications. Here we demonstrate, for the first time, thermally driven resistive switching in thin films of semiconducting CPs consisting of silver ion and tetracyanoquinodimethane ligand (AgTCNQ). High-quality and highly hydrophobic thin films of Ag-TCNQ were fabricated through a layer-by-layer approach upon sacrificing a pre-deposited layer of Cu-TCNQ on a thiolated Au substrate. Reversible switching between the high-resistance state (HRS) at 300 K and the low-resistance state (LRS) at 400 K with an enhancement factor of as high as $\sim 10^6$ in the electrical resistance was realized.[1] The phenomenon is attributed to the alternation of the Schottky barrier at the metal−semiconductor interface by thermal energy and not due to the formation of a conductive filament. Our discovery of thermally driven resistive switching as well as sacrificial growth of CP thin films on an organically modified substrate holds promise for the development of solution-processable non-volatile memory devices.

Keywords: Coordination polymer, Resistive switching, Schottky barrier.

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DOI: https://dx.doi.org/10.5281/zenodo.1170846

Modulation of Electrical Conductivity in Coordination Polymers by Heterometallic Design

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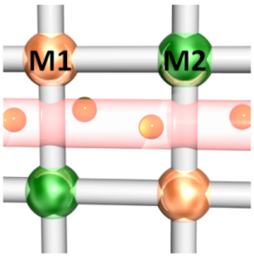
Abstract

Electrically conductive metal−organic coordination polymers (CPs) are promising candidates for a variety of technological applications. However, poor energetic and spatial overlap between the sp-electrons of organic ligands and the d-electrons of metal ion often blocks an effective charge transport (mobility) across CPs. Herein, we present a bimetallic design principle for enhancing carrier mobility in CPs. Bimetallic CPs of Fe(III) and Cr(III) ions coordinated to 1,3,5-benzenetricarboxylic acid (BTC) ligand (Fe−BTC−Cr) exhibited remarkably high carrier mobility at the matching mole ratio (1:1) with enhancement factors of 10^2 and 10^4 in comparison to those of monometallic parents, Fe−BTC and Cr−BTC, respectively. The observation was substantiated by lowering of the band gap between the valence band and the conduction band upon the formation of a hybrid p−n-type structure in the bimetallic CPs. Our flexible approach of picking and choosing the appropriate combination of metal ions from the periodic table is expected to generate various CPs with desirable semiconducting properties.



Keywords: Metal organic coordination polymer, Electrical Conductivity, p-n structure

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DOI: https://dx.doi.org/10.5281/zenodo.1170860

Control synthesis of iron nanoparticle and iron/graphene nanocomposites

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Abstract

Metal nanoparticles show distinct physical, chemical properties from their bulk counterparts due to higher surface to volume ratio and play major roles in various applications such as optical, electrical, thermal etc. Additionally, Graphene has been one of the most investigated 2D materials in last decade due to their excellent electronic, optical and chemical properties. Therefore in the present work to study the metal naoparticle/graphene nanocomposite, we have investigated the optical properties of iron nanoparticles and their composite with graphene. In this work, we have demonstrated successful synthesis of Iron nanoparticles (dimensions ~ 10-15 nm) by room temperature chemical synthesis route. Further, reduced graphene was synthesized by reduction of graphite oxide and iron nanoparticles were decorated on its surface by chemical route to form iron/graphene nanocomposite. Synthesized samples were characterized using XRD, SEM and FTIR spectroscopy etc. Optical properties of synthesized samples were studied using UV-visible absorption spectroscopy.

Keywords: Fe Nanoparticles, Graphene, optical properties.

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DOI: https://dx.doi.org/10.5281/zenodo.1170864

VO_2 based Thermochromic Coatings for Smart window Application

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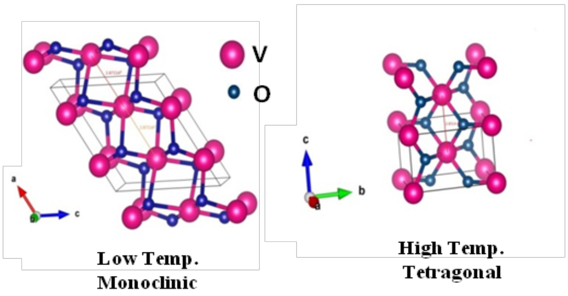
Abstract

Thermochromic (TC) smart coatings are promising for modulating solar radiations. A TC window can be used to automatically control the temperature inside the buildings. Vanadium dioxide (VO_2) was found to be a potent material for technology with a reversible phase transition from monoclinic to tetragonal in somewhat near ambient temperature. However, its use is constrained by low visible transmission (T_{lum}) and high transition temperature (T_c). We achieved a favorable combination of lower T_c , higher ΔT_{sol} and higher T_{lum} by a controlled co-doping of VO_2 with tungsten (W). We adopted a solution processing method that has the advantage of lower cost and easier processability compared to typical vacuum techniques. The precursor is prepared from the V_2O_5 powder and spin coated on the quarts substrate followed by one step annealing at 550^0C in Ar. flow. The major aim of the work is to reduce the transition temperature near 24-30°C and modulate the NIR throughput for window application. Annealing conditions play major role for creating monoclinic VO_2 phase. The produced monoclinic phase shows 43% contrast at 2500 nm with a 25% T_c reduction which is comparable to the other research works.

Keywords : VO_2, solar modulation, co-doping , Thermochromism



Low Temp. Monoclinic

High Temp. Tetragonal

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DOI: https://dx.doi.org/10.5281/zenodo.1170866

Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials

Structural and optical band gap analysis of Mo-modified $PbTiO_3$ ceramics

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Abstract

Perovskiteoxides have beenrecently supposed to be attractive class of materials for use in photovoltaic devices to harvest light energy with various functional properties(1). The spontaneous polarization in ferroelectric perovskite oxides promotes the desirable separation of photo-excited carriers (1).Modoping restricts the recombination rate by charge transfer mechanism promising better optical performance (2). In this attempt $Pb(Mo_xTi_{1-x})O_3$ (x= 0.03 ,0.05 and 0.10) ceramics were synthesized by solid state route. Rietveld refinement of x-ray diffraction patterns reveals that $Pb(Mo_xTi_{1-x})O_3$crystalize into single phase tetragonal structure with space group P4mm.UV-vis spectroscopy measurements shows low band gapbetween conduction and valence band suitable for electron transfer under illumination.

Keywords:X-ray diffraction,Rietveld refinement, UV-Visible spectroscopy, FullProf suite and SEM-EDS.

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DOI: https://dx.doi.org/10.5281/zenodo.1170868

Processing and characterisation of Functionally Graded A356-10wt.%SiC$_p$ Composite

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ABSTRACT

In this paper attempts were made to cast and synthesize functionally graded A356-10wt.%SiC$_p$ composites with circular geometry using liquid stir casting technique followed by vertical centrifugal casting technique. An average particle size of 40 µm was used as the size of SiC$_p$ reinforcement. The microstructure of the composite was examined using Leica optical microscope. The microstructural analysis revealed an outward radial gradient distribution of SiC reinforcement forming different zones and gradation in the distribution of SiC$_p$ particles along the radial direction of the cast disc due to the effect of centrifugal force. Micro hardness values were found to increase in the radial direction of SiC$_p$ distribution.

Keywords:- Functionally graded composite, SiC reinforcement, Microstructure, Micro hardness

DOI: https://dx.doi.org/10.5281/zenodo.1170870

Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India
And National Symposium On Advances In Functional And Exotic Materials

Magnetic Properties of MnAl Alloy with a β-phase

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Abstract

Designing new antiferromagnetic materials is a subject of interest due to their application in spintronic devices without having any stray fields [1-3]. The antiferromagnetic β phase of Mn-Al alloys were synthesized by arc melting followed by annealing. X-ray diffraction along with the Rietveld refinement suggested that these alloys crystallize in a β phase (Space group $P4_132$). The electrical transport data provides an indication of semiconductor-like nature of the alloy. The behaviour of the β Mn-Al alloys was established from the temperature and field dependence magnetization measurement. Moreover, detailed analysis of magnetization data revealed the in-homogenous magnetic disorder in the system with the coexistence of antiferromagnetic and a weak ferromagnetic phase. The strong spin fluctuations in this system lead to a large contribution of the electronic heat capacity [4], whereas the frequency dependent AC-Susceptibility data overuled the possibility of spin glass like behaviour in these alloys. Furthermore, the temperature variation of heat capacity was insensitive to the applied field of 3 Tesla with a negligible magnetic contribution.

Keywords: Intermetallics, Antiferromagnetism, Spintronics, Specific heat, β –Mn phase

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DOI: https://dx.doi.org/10.5281/zenodo.1170874

Effect of gamma irradiation on structural properties of $CrFe_2O_4$ ferrite

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Abstract:

$CrFe_2O_4$ ferrite was prepared by citrate precursor method. Structural properties were determined by X-ray diffraction. Surface morphological and elemental compositions of the prepared samples were studied by high resolution scanning electron microscopy and energy dispersive spectroscopy (EDS). The prepared samples were irradiated to high energy gamma radiation of ^{60}Co source with a dose rate of 6.972 kGy/hr to different doses of 300kGy and 500kGy. The XRD spectra were obtained for the irradiated samples and compared with that of the pristine samples to study the changes in the structure. The obtained results showed that the crystallite size decreases and lattice strain increases with increase of radiation dose.

Key words: chromium ferrite, gamma irradiation, structural changes

DOI: https://dx.doi.org/10.5281/zenodo.1170880

Microstructural and magnetic investigations in Co_2FeGa thin films for spintronics applications

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Abstract:

Half-metallic ferromagnets (HFMs) of Heusler type have drawn great interest due to their predicted high spin polarization at the Fermi level (E_F) [1] and their high potential applications in spintronics such as magnetic tunnel junctions (MTJs) in tunnel magneto resistance (TMR) based devices [2]. Among the Co-based Huesler alloys, Co_2FeGa thin films attracted a great interest due to their high temperature stability. Though Co_2FeGa is not a half-metallic ferromagnet from the first principles calculations, it exhibited a significant spin polarization of 59% using point contact Andreev reflection (PCAR) technique which was created a great interest to study this system for spintronics applications. In light of above, a thickness dependent investigation has been carried out in Co_2FeGa thin films expecting to give a great insight to use them for device applications. The role of film thickness on the structural, microstructural and magnetic properties of Co_2FeGa thin films were systematically investigated. The increase in film thickness shows a linear dependence with grain size. A gradual decrease in coercivity (H_c) and almost constant saturation magnetization (M_s) has been observed at room temperature for the films with grain size > 12 nm. Curie temperature (T_C) is found to increase gradually with increase in grain size. The decrease in H_c and increase in T_C are attributed to the increase in grain size. Temperature dependent magnetic hysteresis loops which exhibit nearly a constant M_s value till 873 K for films of thickness > 10 nm, evidences the high temperature stability of Co_2FeGa thin films. The threshold film thickness to exhibit better thermally stable magnetic properties was identified.

Keywords: Spintronics, Co_2FeGa thin film, microstructure, magnetic property.

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DOI: https://dx.doi.org/10.5281/zenodo.1170882

Optimization of the synthesis and characterizations of chemical bath deposited Cu Doped ZnS thin films

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Abstract

A cost effective chemical route is used to synthesize ZnS: Cunanocomposites. Zinc Sulphide is an important II-VI group semiconductor material possessing superior physico-chemical and optoelectronic characteristics like wide band gap, high chemical stability, large electrochemical coupling coefficient and good photochemical capacity. Further, transparent and conducting ZnS films have found various applications in optoelectronic technology due to its suitable optical, electrical and structural properties. Band gaps were determined using optical absorption measurements and carrier transport properties using conductivity measurements. The thickness of these films was controlled by changing the dipping times and the concentrations of the reaction solution. Experiments showed that the growth parameters and thermal treatment influenced the structure, the morphology and the optical properties of ZnS: Cu films. Structure properties of the films were measured using X-ray diffraction and scanning electron microscopy in the as-deposited and annealed state. The result shows that thermal annealing promotes the growth of grains, decreases band gap, and enhances electrical conductivity

Keywords: Thin films; chemical bath deposition; Structure; Optical properties

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DOI: https://dx.doi.org/10.5281/zenodo.1170888

Controlled Synthesis of Hierarchical Porous Ag_3PO_4 Microspheres through Natural Template for Photocatalytic Applications

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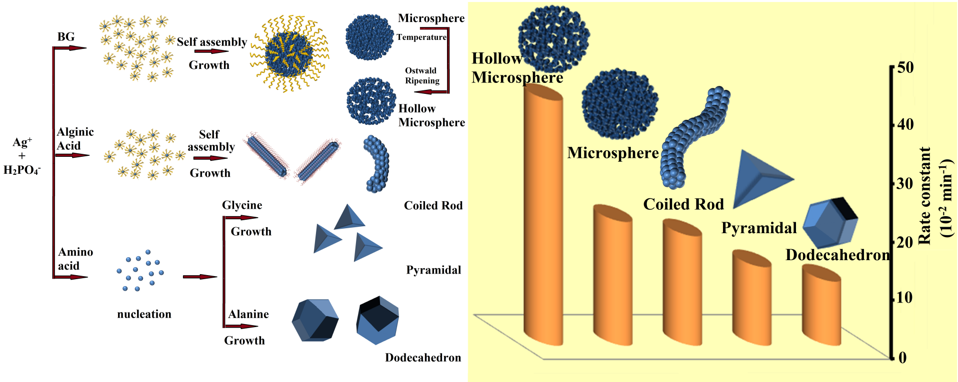
Abstract

Controlled synthesis of targeted morphologies in nanoscale is a challenging field for material chemists. Strategic methods would be required to obtain hierarchical porous semiconductors with specific morphologies or controlled porosities for surface applications. In the recent years, Ag_3PO_4 is considered as a useful material for semiconductor photocatalysis. There are many researchers attempted for the synthesis of these materials; however, Ag_3PO_4 having very high surface area is on the demand. In this work, we tried to achieve uniform hierarchical Ag_3PO_4 porous microspheres through natural bone glue (BG)-assisted one-step precipitation reaction at room temperature. We investigated the effect of supporting parameters (such as BG content, template constituents, temperature, reaction time, etc.) in tuning the morphology, porosity or size of Ag_3PO_4. Photocatalytic capacity of the prepared material was established on the degradation of RhB and 2,4 DCP under visible light, which was found to be significantly better than other architectures. The method demonstrated would pave the way for development of porous hierarchical nanomaterials for various applications.



Scheme: Synthesis of hierarchical porous Ag_3PO_4 microspheres and their superior photocatalytic activity over other architectures.

Keywords: Bone glue, Rhodamine B, 2,4-Dichlorophenol, Photocatalysis, Visible light.

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Mandal, S.; Ananthakrishnan, R. *ACS Sustainable Chem. Eng.* (Just accepted) DOI:10.1021/acssuschemeng.7b03391

DOI: https://dx.doi.org/10.5281/zenodo.1170892

A comparative study on in-vitro bioactivity of nano-Bioglass synthesized using rice husk and TEOS silica sources

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Bioactive glasses bond to living tissues and, for thisreason, they have been studied for their use in differentclinical applications, mainly in the field ofbone repairand replacement: filling ofosseous cavities, manufacturingof small parts ofmiddle ear bone replacement,maxillofacial reconstruction and dental applications. Different bioactive glass and glass ceramics have been synthesized in order to get desiredmechanical, chemical properties by obtaining required microstructure. Some of commoncomponents used are Na_2O, CaO, P_2O_5, SiO_2 for synthesis of a unique highly compatible 45S5 Bioglass system. In general, Bioglass has shown higher compatibility when synthesized by sol-gel route compare to melt casting method. Various in-vitro studieshave shown that the nucleation and crystallization ratesofhydroxycarbonate apatite (HCA) depends on manyfactors including the sol–gel glass composition.

In the present work, in order to reduce the cost of Bioglass and also enhance the bioactivity of Bioglass a study has been done to synthesis Bioglass from risk husk and TEOS as silica sources. Sintering and crystallization phenomena in powders of a typical bioactiveglass composition (45S5 Bioglasss) have been investigated in order to gainfurther understanding of the processes involved in the fabrication ofBioglasss based glass–ceramic scaffolds for tissue engineering applications.To assess the in vitro performanceand bioreactivity of Bioglasss-derived glass–ceramic scaffolds, thebiodegradation of samples in simulated body fluid (SBF) was investigatedusing various techniques, including SEM, XRD and EDX.

Keywords: Bioglass, Rice Husk, Bioactivity

DOI: https://dx.doi.org/10.5281/zenodo.1170894

Influence of H^+ ions and γ-ray irradiation on multiferroic $Bi_{0.8}Ca_{0.2}MnO_3$ thin films

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Abstract

Polycrystalline Multiferroic materials having coupled electric, magnetic and elastic orderings provide a platform for memory and logic devices. Controlling polarization switching mechanisms in ferroelectric and multiferroic materials is a critical step towards the oxide-based electronic devices including data storage devices, tunneling barriers and field-effect transistors. Bismuth manganite ($BiMnO_3$) has been regarded as one of the prominent multiferroic materials. Here $Bi_{0.8}Ca_{0.2}MnO_3$ (BCMO) thin films were deposited on Si (100) substrate using RF magnetron sputtering. The grown films have been subjected H^+ ions and γ- ray irradiation to enhance its magneto electric coupling for memory devices. Moreover, the structural, elemental, magnetic and electrical properties of these irradiated BCMO films have been analyzed.

Keywords: $Bi_{0.8}Ca_{0.2}MnO_3$ thin films**,** sputtering, ferroelectricity, ferromagnetism

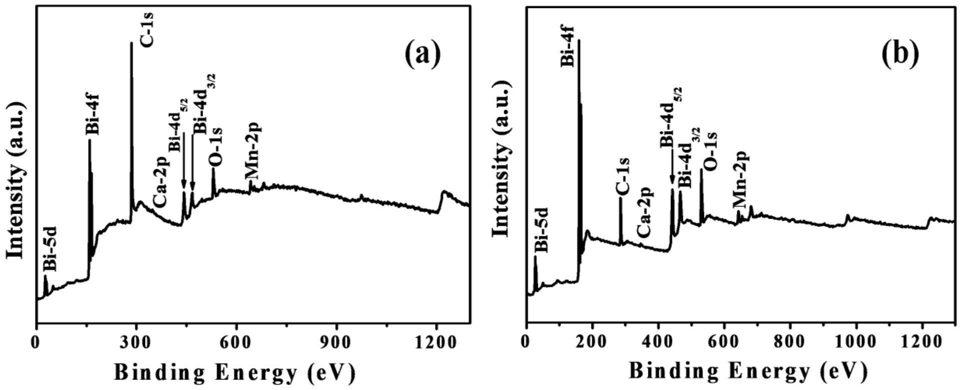

Figure: XPS survey spectra of (a) H^+ ions irradiated (b) γ-ray irradiated $Bi_{0.8}Ca_{0.2}MnO_3$ film

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DOI: https://dx.doi.org/10.5281/zenodo.1171073

Magnetic properties of aluminum doped Barium Hexagonal Ferrite

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Abstract

$BaAlFe_{11}O_{19}$ nanoparticles were synthesized by modified sol gel autocombustion method and were subsequently annealed at different temperatures. Structural studies showed the presence of single phase $BaAlFe_{12}O_{19}$ in the samples annealed at and above 900ºC. The average grain size was found to be increased after annealing. The spontaneous magnetization (M_s) value shows systematic variation with the increase in annealing temperature. Maximum values of 71 and 109 emu/g were observed at 300K and 60K respectively for the sample annealed at 1200°C. A maximum coercivity of 6696Oe was observed at 300K for the sample annealed at 1100 ºC. Magnetization was increased at 60 K compared to that at 300 K whereas the coercivity decreased for all the annealed samples at 60 K. The observed magnetization behaviour in these nanoparticle samples may be explained on the basis of grain growth, canting of moments, modified exchange interactions in the lattice.

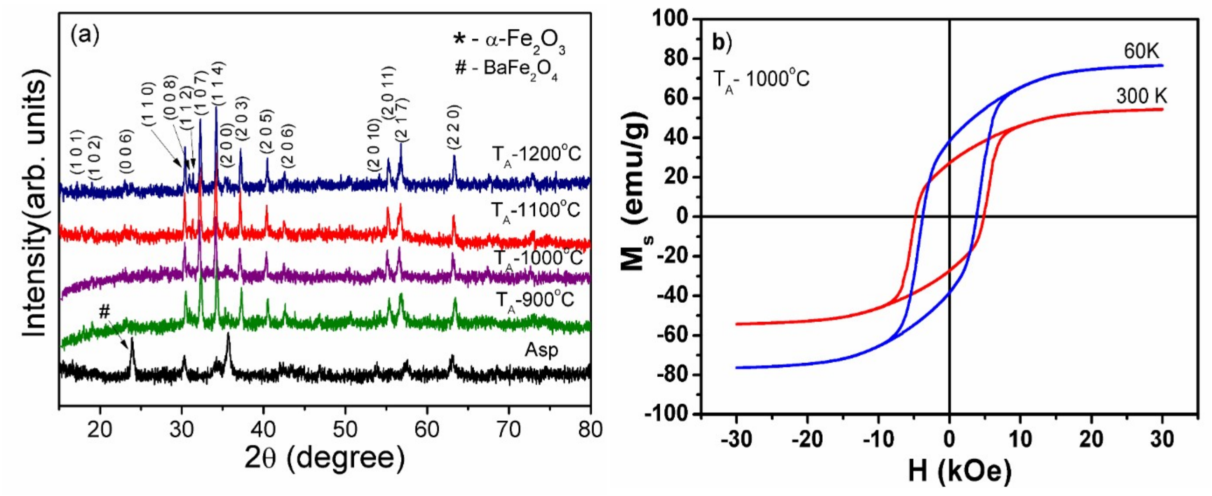

Fig.1. a) XRD patterns of the BaF-Asp and samples annealed at different temperatures b)Typical M-H loops of the T_A-1000 sample at 300K and 60K.

Keywords: sol gel autocombustion,exchange interactions and canting.

DOI: https://dx.doi.org/10.5281/zenodo.1171081

Structural and spectral studies of 4-methylbenzylammonium nitrate crystal

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Abstract

An organo-inorganic hybrid crystal fabricated from 4-methylbenzylamine cations and NO_3 anions has been synthesized by slow evaporation solution growth method. The single crystal X-ray diffraction method was employed to determine the structural parameters. It is found that the crystal belongs to monoclinic crystal system with space group $P2_1/c$. The unit cell parameters were also determined. The UV-Vis-NIR spectrum established the optical transparency and the lower cut off wavelength is found to be 230 nm. The vibrational modes of various functional groups are found by FTIR spectrum. The molecular structure of the title compound was established by ^1H and ^{13}C NMR spectroscopy.

DOI: https://dx.doi.org/10.5281/zenodo.1171085

Superconducting properties of tungsten meander structures fabricated by focused ion beam technique

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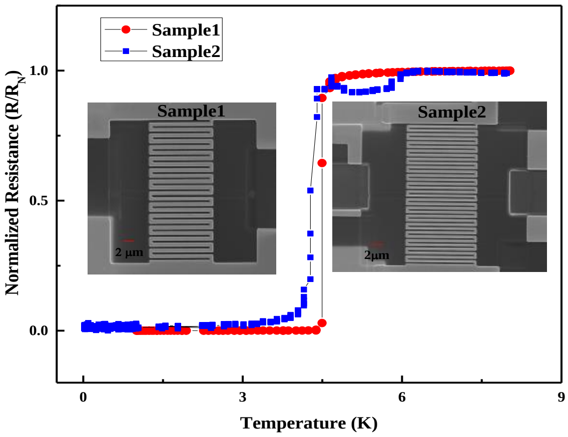
Abstract

Focused ion beam (FIB) deposited tungsten is reported to have a superconducting transition temperature of ~5 K (1), as it forms an amorphous alloy comprising of W, Ga and C. Here we report the fabrication and superconducting characteristics of meander structure of tungsten deposited by FIB technique. Two such structures were fabricated with varying width ~ 450 nm (sample1) and ~300 nm (sample2). The superconducting transition temperature of sample1 is 4.5 K and that of sample2 is 4.3 K, which were measured in the Dilution Refrigerator having a base temperature of 20 mK. While the R(H) characteristics of Sample1 is of a typical type-II superconductor, sample2 shows some anomalies including resistance oscillations, the H_{C2} values of both the structures is estimated to be ~9.5 T. The figure given below shows the variation of normalized resistance as a function of temperature along with SEM image of the meander structures.



Keywords- Superconductors, FIB, Dilution Refrigerator, meander structure

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DOI: https://dx.doi.org/10.5281/zenodo.1171087

Structural, linear and nonlinear optical studies of 4-methoxybenzylammonium tetrachloridozincate crystal

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Abstract

A semiorganic nonlinear optical 4-methoxybenzylammonium tetrachloridozincate (4MBAT) crystal has been grown by slow evaporation solution growth technique. Single crystal X-ray diffraction (XRD) study was carried out to determine the lattice parameters of 4MBAT crystal. XRD result revealed that 4MBAT crystal belongs to monoclinic crystal system with non centrosymmetric space group $P2_1$. UV-Vis-NIR transmission spectrum was recorded to analyse the optical characteristics. The transmission spectrum exhibit a good optical transmittance up to 1100 nm with the UV absorption edge at 271 nm. ^{1}H and ^{13}C NMR spectral studies established the molecular structure of 4MBAT crystal. The second harmonic generation (SHG) test was performed to know SHG efficiency of the 4MBAT crystal using Kurtz-Perry powder method. The nonlinear optical efficiency of 4MBAT is 1.8 times higher than the standard potassium dihydrogen phosphate (KDP).

DOI: https://dx.doi.org/10.5281/zenodo.1171094

Electron Beam Lithography of sensitive resist based on photoacid generator integrated terpolymer: potentiality of high-resolution pattern transfer

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Nanolithography technology has been extensively used in semiconductor fabrication process to manufacture micro/nano electronics. Now a days developing new photoresist materials for different lithography applications in successful pattern transfer has been the key role in semiconductor industries for next-generation IC technology node. On these note, we have designed and synthesized a new terpolymer viz. GBLMA-MAMA-MAPDST photoresists for the electron beam lithography (EBL) applications (1, 2). EBL studies reveal that the synthesized terpolymer resist (GBLMA-MAMA-MAPDST) is sensitive to the e-beam with 100 nm (L/S) and 70 nm isolated positive tone line features after TMAH development. The terpolymer resist showed remarkable sensitivity (E_0) and contrast ratio (γ) of ~36.5 µC/cm^2 and ~0.08, respectively. Eventually, the potential to transfer positive higher resolution nano-features on the silicon substrate has been demonstrated by suitable dry plasma etching technique.

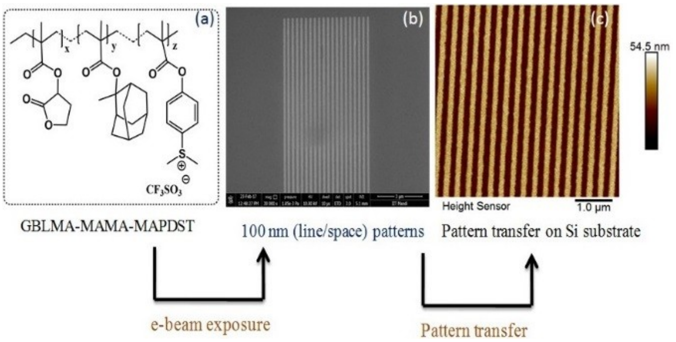

Fig. 1. (a) Structure of Terpolymer, (b) EBL pattern of 100 nm L/S, (c) AFM image of transferred pattern onto Silicon.

Keywords: EBL, Integrated Terpolymer, Pattern Transfer, Sensitive Resist.

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DOI: https://dx.doi.org/10.5281/zenodo.1171217

Synthesis and characterization of (1-x) $BaTiO_3$ – $xCoFe_2O_4$ - Multiferroic composite

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Abstract

Recently, much attention has been paid to the investigation of multiferroic composite materials which have a combination of two or more materials with ferroelectric (e.g., $BaTiO_3$ and $PbTiO_3$), ferromagnetic (e.g., $CoFe_2O_4$ and $NiFe_2O_4$) and show magnetoelectric (ME) coupling effect [1].These materials areattractive because they offer the possibility to control the polarization by a magnetic field or the magnetization by an electric field. The coupling effects provide multiferroic composites in the applications like electro-magnetic interference filters, capacitors, transducers, and integral chip inductors [2-4]. In present study, (1-x) BaTiO3– $xCoFe_2O_4$ (x=0.00, 0.05, 015) ceramics have been synthesized by a solid-state reaction route. Formation of the composite with two separate ($BaTiO_3$ – $CoFe_2O_4$) phaseshave been identified by X-ray diffraction (XRD) analysis. The leakage current density (J-E) is found to be increased with the increase of $CoFe_2O_4$concentration while varying at different electric field.

An enhancement of magnetization with increasing $CoFe_2O_4$concentration has been observed at room temperature magnetization studies using vibrating sample magnetometer (VSM). Polarization versus electric field (P-E) hysteresis loops show that, the ferroelectric properties decreases with increasing $CoFe_2O_4$content. Further, the temperature dependent dielectric constant measured for BTO/CFO ceramic samples at different frequencies and magneto electric coupling studies have also been performed. The details of the results will be presented and discussed.

Keywords: **Multiferroic, BTO/CFO, Magneto –dielectric, solid state reaction.**

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DOI: https://dx.doi.org/10.5281/zenodo.1171226

Synthesis, growth and characterization of R-Mandelic acid S-alanine hemihydrates single crystals

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Abstract

Nonlinear optical (NLO) active single crystals of R-Mandelic acid S-alanine hemihydrate (RMSA) were grown by solvent evaporation procedure at 37°C. The lattice constants were determined by single crystal and powder X-ray diffraction analysis. RMSA crystallizes in triclinic structure. Transmission spectrum of RMSA shows the UV cut-off wavelength at 268 nm. The vibrations of functional groups were elucidated by FTIR spectroscopy. The molecular structure of RMSA was established by ^{13}C-NMR spectroscopy. Kurtz–Perry SHG test showed positive results for SHG. The SHG efficiency is found to increase for RMSA when compared to pure alanine. Third order nonlinear optical study was carried out using single beam Z-scan technique using He-Ne laser. Closed aperture study reveals the positive nonlinearity in RMSA and open aperture study reveals the reverse saturation absorption of the grown crystal.

DOI: https://dx.doi.org/10.5281/zenodo.1171230

High pressure and dielectric properties of the spin-½ compounds Ba_2CuTeO_6

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Ba_2CuTeO_6 compound exhibits two phases, one is prepared at ambient pressure and other can only be synthesized under high-pressure. Sample prepared at 900^0C under 6 GPa pressure crystallizes in a perovskite type structure (Fig. 1). Whereas samples prepared at ambient pressure crystallizes in triclinic structure (Fig. 1) and also show structural transition T_S around 285 K. In triclinic two-leg spin ladders are formed by the tellurium-bridged Cu^{2+}(S = ½) ions. With decreasing temperature, $\chi(T)$ curve displays a broad maximum at 75 K with the subsequent drop and then a small kink at T_N = 15 K. In addition, the real part dielectric constant $\varepsilon'(T)$ exhibit a frequency independent peak near the structural transition temperature T_S (Fig. 2). Since the dielectric properties are very sensitive to the local electric field distribution of the samples, studies of the temperature and frequency dependent dielectric behavior can provide us a better understanding about the magnetic/structural transition of this compound.

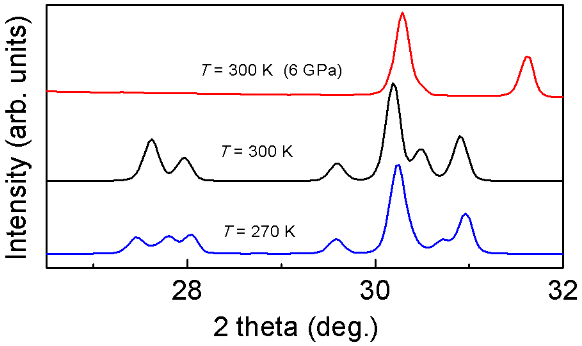

Fig. 1 X-ray diffraction of Ba_2CuTeO_6 compounds.

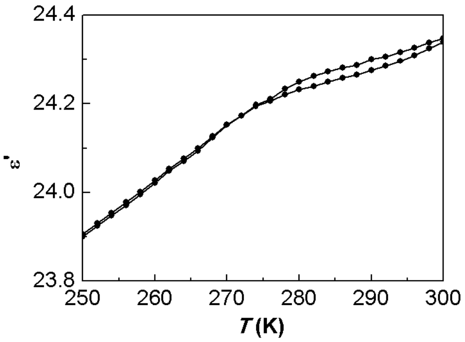

Fig. 2 Real permittivity vs temperature.

Keywords: Perovskite, High pressure, real permittivity, spin ladders.

DOI: https://dx.doi.org/10.5281/zenodo.1171234

Effect of Pressure on superconducting properties of endohedral gallide cluster based superconductor Mo_8Ga_{41}

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Endohedral gallide cluster is found to be a structural motif that favors existence of superconductivity. Some of the examples are Mo_8Ga_{41}, Mo_6Ga_{31}, $ReGa_5$, $PuCoGa_5$[1-3]. We synthesized Mo_8Ga_{41} superconductor that shows superconducting transition at 9.8 K. The upper critical field (H_{c2}), lower critical field(H_{c2}), coherence length(ξ) and penetration depth(λ) are found to be 11.8T, 150G, 5.2nm and 148nm respectively. On applying pressure(0-1.1GPa) the transition temperature decreases from 9.8 to 9.6 K while almost two fold enhancement in critical current density(J_c) is evaluated from M-H loop taken at 2K ($\sim 10^5$A-cm^{-2}). Similar enhancement in J_c was also estimated from M-H loop taken at 7K and 9K. The Kramer's fitting for normalized pinning force F_p vs. reduced field ($h=H/H^*$), where H^* is irreducible field yields the presence of multiple pinning mechanism based on point, surface and volume pinning. The double exponential model fitting on J_c vs. reduced field h indicates two gap superconductivity[4].

Keywords: Superconductivity, Pinning, Critical current density, Pinning force density.

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DOI: https://dx.doi.org/10.5281/zenodo.1171240

Effect of processing parameter on the structure and magnetic properties of barium hexaferrite sputtered thin films

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Abstract:

In the present work, high coercivity barium hexaferrite (BaM) thin films were fabricated by RF sputtering. The effect of film thickness, annealing temperature and Argon pressure on structural and magnetic properties were investigated by X-Ray diffraction pattern (XRD), Scanning electron microscope (SEM) and Vibrating sample magnetometer (VSM). Diffraction pattern confirms thickness and post annealing temperature are the two major parameters for better crystallization. SEM micrograph shows highly dense uniform films were obtained by lower argon pressure. Higher coercivity and squareness were obtained for one hour sputtered BaM thin film.

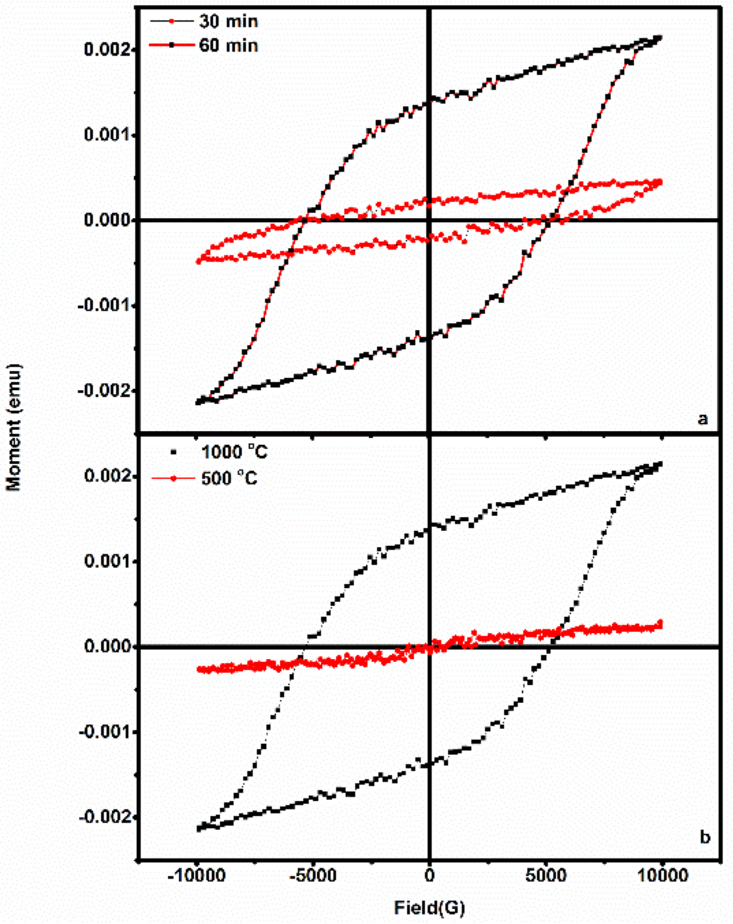

Fig. M-H plot for barium hexaferrite thin film

DOI: https://dx.doi.org/10.5281/zenodo.1171242

High-level supercapacitive performance of chemically reduced graphene oxide

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Abstract: Commercial supercapacitors, mainly made of activated carbon, offers insufficient capacitance at high cost. Recently, graphene-based materials are emerging as smart alternatives. Reduction of graphene oxide (GO) is an elegant and important approach to produce reduced graphene oxide (rGO), because it holds the promise to closely resemble its physicochemical properties with pristine graphene. The conventional reducing agents such as sodium borohydride and hydrazine are strong reducing agents, and cannot be recycled. The fast reaction kinetics bring an imbalance in the desirable properties of rGO. Here, we present one-pot chemical reduction of GO in aqueous medium by an unconventional mild reducing agent ($FeCl_2$/HCl) where pure rGO is isolated and the reducing agent is recycled upon simple treatment of the filtrate with HCl. The fabricated all-solid-state supercapacitor of as-synthesized rGO exhibited significantly higher specific capacitance (171 F/g at 1.1 A/g), remarkable cycling stability (>80% retention of capacitance beyond 100,000 continued cycles), and flexibility (>500 bending cycles), which is comparatively better than those of rGO derived from conventional reducing agents. Use of commercially available organic electrolyte further boosted the supercapacitor performance (282 F/g at 1.8 A/g) of rGO.[1]

Keywords: chemical reduction, reduced graphene oxide, all solid-state supercapacitor, durability

Reference

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DOI: https://dx.doi.org/10.5281/zenodo.1171244

New Emerging Rare-Earth Doped Luminomagnetic Nanorods for Cellular Imaging Applications

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Abstract

Nanoparticles possessing, both, magnetic and photoluminescence features in a single host lattice have an exceptional utility in multimodal cellular imaging. We have synthesized bifunctional luminomagnetic $Gd_{2-x}Eu_xO_3$ (x = 0.05 to 0.5) nanorods, with a diameter of ~20 nm and length in ~0.6 μm, using hydrothermal method and characterized for its structural, optical and magnetic properties (1). These as synthesized luminomagnetic nanorods exhibit hypersensitive red emission (610 nm) and paramagnetic properties. The cytotoxicity analysis of these nanorods with two human breast cancer cell lines T47D and MDA-MB-231 shows its utility in biomedical applications. Further, the cellular imaging capabilities *in vitro* and *in vivo*, of these luminomagnetic nanorods were also investigated by T47D and MDA-MB-231 cell lines. Moreover, we have also compared the photoluminescence and paramagnetic characteristic of $Gd_2O_3:Eu^{3+}$ nanorods with the spherical nanoparticles of $Gd_2O_3:Eu^{3+}$, to understand the significance of shape of the nanostructure. Hence, these as synthesized luminomagnetic nanorods provides highly biocompatible nanoprobes for cellular imaging applications.

Keywords

Luminescent, Magnetic, bifunctional, cellular imaging, *invitro, invivo*

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Gupta, B. K. *et al.* Bifunctional Luminomagnetic Rare-Earth Nanorods for High- Contrast Bioimaging Nanoprobes. *Sci. Rep.* 6, 32401

DOI: https://dx.doi.org/10.5281/zenodo.1171252

Superconductivity of high density nonmagnetic cobalt

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Metals possessing strong long-range magnetic order, as in antiferromagnetism or ferromagnetism, do not exhibit superconductivity [1]. This includes ferromagnetic transition metals Fe, Co and Ni. However, some elements, which do not show superconductivity under ambient pressure, become superconducting under higher pressure. Fe has been found to undergo a superconducting transition at pressures between 15 and 30 GPa with a critical temperature (T_c) of about 2 K [2]. Fe is nonmagnetic at this pressure. Superconductivity was not hitherto observed in Co and Ni under any condition. Recently, a high-density nonmagnetic (HDNM) face-centered cubic (*fcc*) phase of Co was discovered in Co thin film [3]. As this phase of Co is nonmagnetic, one can expect superconductivity in this HDNM phase of Co. We have indeed discovered superconductivity in the high-density nonmagnetic Co thin film with a superconducting transition temperature (Tc) of ~9.5 K and a critical field (Hc) of ~ 35 kG [4]. The transition to the superconducting state has been detected by point-contact spectroscopy and drop in resistance in point contact measurements as well as in standard four probe resistivity measurement method. In 4-probe method the transition temperature is ~5.4 K. This difference in transition temp could be due to strain distribution over the film since the strain is playing the key role. First-principles density functional theory calculations for this dense *fcc* phase of Co show that this phase is nonmagnetic and the estimated T_C within the BCS theory is 0.30 K. A volume preserving strain in *fcc* Co is shown to result in anomalous softening of zone boundary phonons which couple strongly with electrons, and stabilize superconductivity at a relatively large temperature (>5 K). The value of T_C can indeed be higher for other strain conditions.

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DOI: https://dx.doi.org/10.5281/zenodo.1171256

Structural, Dielectric, Vibrational and Semiconducting Properties of Ferroelctric-Photovoltaic $Bi(Ni_{1/3}\ Nb_{2/3})O_3$-$PbTiO_3$ material

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In this study, We demonstrate the development of (1 -x)$Bi(Ni_{2/3}Nb_{1/3})O_3$–x$PbTiO_3$ (BNN-PT) samples with composition (x=0, 0.77, 0.70, 0.65, 0.625, 0.60,0.55) using the conventional solid-state reaction technique .

Phase identification and structural characterization of sintered BNN-PT powders for all compositions were made by X-Ray diffraction technique. The Optical, structural, magnetic, ferroelectric and dielectric properties were measured for all compositions. The Raman mode A1 shifts to lower frequency and the average grain size decreases with BNN doping which is due to difference in ionic radii of Ti and Ni. The ferromagnetic properties of BNN-PT improved with increasing the doping concentration of Ni. The optical band gap reduced from 3.0 eV to 2.1 eV with varying the BNN doping in BNN-PT. It is observed that band gap of BNN-PT depends on doping percentage of Ni. The reduced band gap makes the BNN-PT promising material for ferroelectric photovoltaic applications.

Keywords: X-ray diffraction, Perovskite, Photovoltaic, Ferro-electric.

DOI: https://dx.doi.org/10.5281/zenodo.1171260

Tuning the morphology and structure of vertical graphene nanowalls: Raman and EELS study

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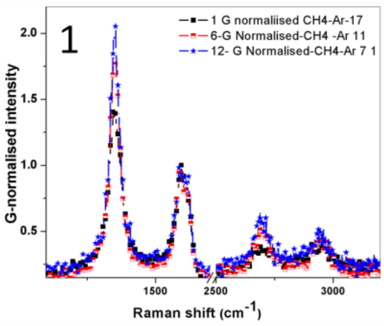
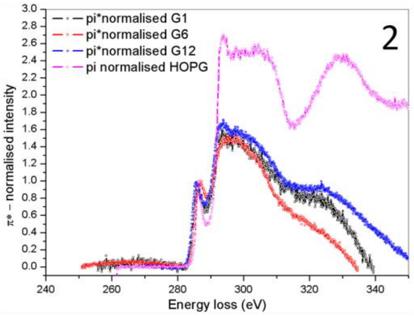
Abstract

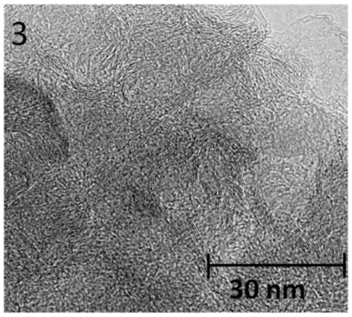
The influence of process gas composition on the morphology and structure of vertical graphene nanowalls (VGNs) deposited by plasma enhanced chemical vapour deposition (PECVD) is studied. Argon percentage was systemically varied against methane under similar process conditions. Both morphological and structural variations were revealed from SEM and Raman studies. The crystallite size calculated from ID/IG ratio showed a direct correlation with increase in methane concentration. The ID/ID' ratio was correlated with gas mixture to infer the characteristics of defects in VGNs. In concurrence with SEM and Raman study, 'a few layer graphene' structure was revealed from TEM analysis. Selected area diffraction pattern showed nanocrystalline nature of VGNs and decrease in d-spacing with increase in methane concentration. In the low loss region of electron energy loss spectroscopy (EELS), σ* plasmon showed a minimum at 1:1 gas ratio, whereas π* Plasmon became more graphitic with increase in methane concentration. A lower fraction of sp2 type bonding was observed for 1:1 concentration in the high loss region[1]. The present study showed that inert Argon can be effectively used for tuning the plasmonic properties of VGNs towards better super capacitor, field emission, catalytic and fuel cell applications.



1. G-normlised Raman spectra showing variation of D-band int. with composition



2. Π* normalised EELS spectra of VGNs **and HOPG for** sp2 percentage calculation



3. HR TEM image showing the few Layer VGNs

Key words: PECVD, VGNs, Raman spectroscopy, EELS

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DOI: https://dx.doi.org/10.5281/zenodo.1171264

Design and synthesis of “AIEE” luminogen, modified itto “AIE”luminogen by small modification and used forlatent fingerprint imaging

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Abstract

Latent fingerprints (LFPs)has various whorls, arches and loops that are identical for a person. As a result almost a century fingerprints used as a means of identification (1). Aggregation inducedemission (AIE) luminogens are highly fluorescent in nanoparticle form and solid statebut less or not fluorescentin the soluble state. Classical luminogensshow opposite properties then AIE molecules, these molecules are calledaggregation causedquenching (ACQ)molecules.There are some luminogens they show higher emission in semi aggregated state they are called aggregation induced enhance emission(AIEE) luminogens (2).So keeping benefits of AIE molecule we synthesizedTPBZ and TPBC.We used it for latent fingerprintimaging on different substrates. TPBZ and TPBC characterized by MALDI-TOF, ^{1}HNMR,^{13}C NMR and nanoparticles studied by DLS spectroscopy.

Keywords: **AIE, AIEE, Latent fingerprint imaging**.

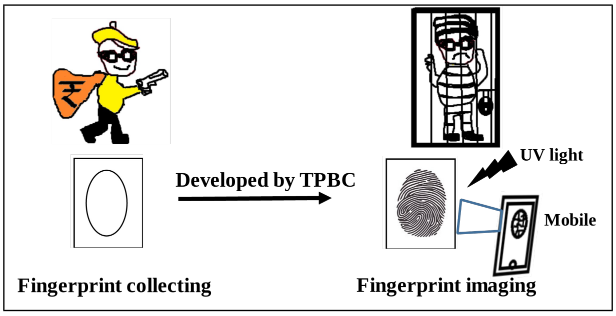

Fig. Pictorial representation of visualization of LFPs by TPBC

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DOI: https://dx.doi.org/10.5281/zenodo.1171266

Magnetic and Impedance Spectroscopy Studies in Mg Doped Barium Hexaferrite

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Abstract

Y-type hexaferrites have attracted an extensive research interest due to their potential applications in electronic and microwave devices [1-2]. Polycrystalline Mg-doped $Ba_2(Co_{1-x}Mg_x)_2Fe_{12}O_{22}$ ($0 \leq x \leq 1$) samples are found to be in single phase form and their crystal structure, magnetic and dielectric properties arestudied.The saturation magnetization (M_s)values are found to decrease from 27 emu/g for $x = 0$ to 20 emu/g for $x = 1$ samples. Similarly the coercivity (H_c) values are found decrease with increase in Mg concentration.The temperature dependence magnetization measurement shows that the Curie temperature decreases from 613K for x=0 to 535K for $x = 1$.Impedance spectroscopy measurements at different temperatures exhibitrelaxation peaks due to grains and grain boundaries contributions. The analysis of ac conductivity data in terms of Jonscher power law suggests that the underlying conduction mechanism is controlled by small polaron hopping.The activation energy for conduction is found to decrease with Mg doping from 0.77eV for $x = 0$ to 0.23eV for $x = 1$.The detailed analysis of magnetic and impedance spectroscopy studies and the underlying physical mechanism would be presented.

Keywords: Mg doped Barium Hexaferrite, ac impedance spectroscopy, small polaron hopping,

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DOI: https://dx.doi.org/10.5281/zenodo.1171270

Magnetic and Dielectric Properties of Transition Elements Substituted Yttrium Iron Garnets

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Abstract

Yttrium iron garnet (YIG) is a natural choice for microwave devices [1]. We have successfully prepared polycrystalline samples of transition elements (Cr and Mn) substituted YIG in single-phase form. The lattice parameter is found to decrease with increase in concentration of doped transition elements. Room temperature saturation magnetization value is found to increase with increase in Cr and Mn concentrations. The analysis of impedance spectra shows the deviation of relaxation process from ideal Debye type. In Cr substituted YIG, both grains and grain boundaries are found to contribute while in Mn substituted YIG only grain boundaries are contributing towards the relaxation process. The value of dielectric constant at 1MHz is found to increase with increase in Cr concentration from the value of 20 for $x = 0$ to 52 for $x = 0.5$ while, in case of Mn substituted YIG the dielectric constant is found to slightly decrease to $\varepsilon' = 13$ for $x = 0.2$. These samples show an anomaly in the vicinity of magnetic transition temperature which may be attributed to the magneto-electric coupling.

Keywords: Magnetic ceramics; yttrium iron garnet; saturation magnetization; impedance spectra;

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Incommensurate skyrmionic phase in triangular spin lattice of helimagnet $NiBr_2$

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Abstract

The spin-spiral magnets are an important class of multifunctional material that shows coupling between ferroelectric polarization magnetic orders. The triangular-lattice of antiferromagnetic nickel dibromide ($NiBr_2$) with helical spin structures often exhibits a highly unusual magnetic ordering due to competition between ferromagnetic and antiferromagnetic exchange interactions. Using DC (AC) magnetometry, a detailed investigation of incommensurate skyrmionic phase at low temperature has been carried out. In such helix phase ($T<T_H=23K$) the elliptically disordered spins successfully detected. The strength of disorder can control by varying the temperature as assured by kink shaped magnetic hysteresis loops measured in helix phase ($T<T_H$). These experimental findings are highly significant for the proper understanding of the involved microscopic mechanisms in the precursor stage of incommensurate skyrmions, which has various technological implications for next-generation magnetic memory devices.

Keywords: Helimagnetism, Skyrmion, domain wall, Dzyaloshinskii-Moriya interaction.

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DOI: https://dx.doi.org/10.5281/zenodo.1171278

Structural, magnetic and transport properties of $CeAg_{0.68}Si_{1.32}$ polycrystalline compound

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We report on a comprehensive study on the preparation, structure, magnetization, resistivity and heat capacity of the polycrystalline compound $CeAg_{0.68}Si_{1.32}$. The compound crystallizes in the hexagonal $A1B_2$ type structure with *P6/mmm* space group. Magnetic susceptibility studies reveal two ferromagnetic transitions at 4.6 K and 7.6 K. A small hysteresis loop observed in isothermal magnetization at 2 K indicates a soft ferromagnetic behavior. Reduction in experimental value of saturation magnetization from the theoretical value is attributed to the Crystal Electric Field Effect (CEF). The temperature dependent specific heat capacity exhibits a broad hump at low temperatures (Fig. 1) which may be due to the bulk magnetic ordering. Resistivity data exhibits spin disorder scattering near the ordering temperature. The negative magnetoresistance (-3% at 2 K in 60 kOe) indicates ferromagnetic behavior.

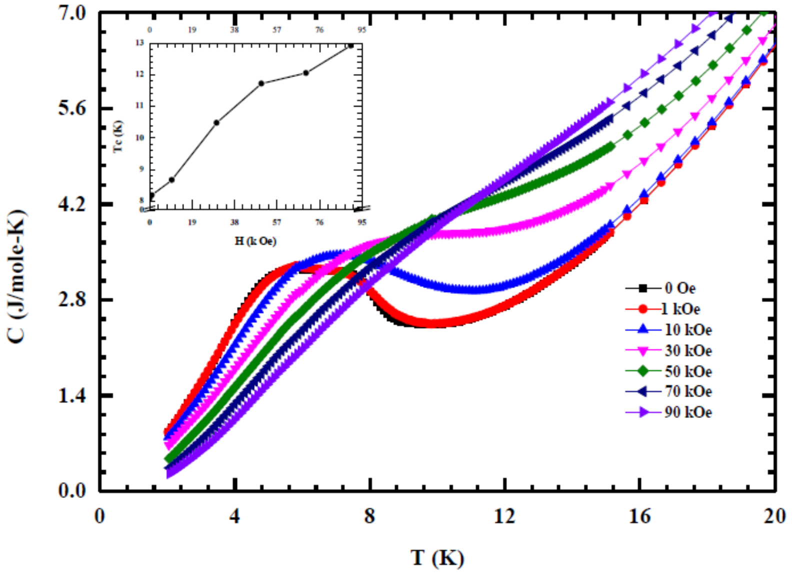

Fig. 1. Temperature dependence of the heat capacity measured in different magnetic fields upto 90 kOe of $CeAg_{0.68}Si_{1.32}$.

Keywords: Rare earth-transition metal compound; Magnetic properties; Resistivity, Heat capacity

DOI: https://dx.doi.org/10.5281/zenodo.1171280

Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials

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Phase transition in potassium hydrogen phthalate crystals –effect of various molar concentration of L-Proline

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Abstract:

This paper Investigate the crystalline nature of potassium hydrogen phthalate by addingL-Proline in three different molar concentrations. The crystals prepared by the slow evaporation method and characterized by Ultraviolet spectrum, Fourier Transform of Infrared analysis and Powder x-ray diffraction techniques. We observed all these materials are good absorption and transmission in UV region. As we calculated the energy that there is a loss of energy due to the inelastic scattering occurs in UV analysis. The Phase transition takes place as we increased the concentration of L-Proline with potassium hydrogen phthalate. For first and third molar concentration, the samples crystalized in orthorhombic system, and for fifth molar concentration the crystals crystallized in monoclinic system. But the crystals have Cmc21, Ibca and C121 space groups for first molar, third molar and fifth molar concentration respectively. Caglioti parameters, particle size, systematic absences were also analysed by powder peak pattern of this crystals. The Size and Strain graph plot of Williamson-Hall plot and crystallite size distribution graph of Warren-Aver Bach method interprets strain coefficient, size coefficient and L graph of (Δd/d)% versus length of peaks pattern predicted by PXRD data.

Keywords: UV-Vis, FT-IR, PXRD, Williamson-Hall Plot, Warren-Aver Bach Method.

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   ISSN 0974-3103 Volume 8, Number 1 (2016), pp. 53-57

DOI: https://dx.doi.org/10.5281/zenodo.1171284

Phase transition in potassium hydrogen phthalate crystals – effect of various molar concentration of L-Glutamine

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Abstract:

This paper Investigate the crystalline nature of potassium hydrogen phthalate crystals when added with L-Glutamine in three different molar concentrations prepared by the slow evaporation method and characterized by Ultraviolet spectrum, Fourier Transform of Infrared spectrum and Powder x-ray diffraction techniques. Calculated energy show that there is a loss of energy due to the inelastic scattering occurs in UV analysis. The phase transitionoccursdue the variation in concentration of L-Glutamine. As the concentration increases the increased concentration changes the crystal system of grown crystals. The cell parameters, particle size, systematic absences analysed by powder peak pattern of this crystals. The Size and Strain graph plot of Williamson-Hall plot and crystalline size distribution graph of Warren-Aver Bach method interprets strain coefficient, size coefficient and L graph of (Δd/d) % versus length of peaks pattern predicted by Powder X-ray diffraction data.

Keywords: UV-Vis, FT-IR, PXRD, Williamson-Hall Plot, Warren-Aver Bach Method.

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DOI: https://dx.doi.org/10.5281/zenodo.1171290

Phase transition in ammonium di hydrogen orthophosphate crystals –effect of various molar concentration of amino acid

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*Corresponding Author Email: sinthi@andavancollege.ac.in, Cell No: 9486732241

Abstract

This paper investigatescrystals of Ammonium dihydrogen orthophosphate after the addition of L- Phenyl Alanine in three different molar concentrations prepared by the slow evaporation method and characterized by Ultraviolet spectroscopy, Fourier transform of Infrared analysis and Powder X-ray diffraction techniques. We observed all these materials have good absorption and transmission in UV region. As concentration increase, there is a decrease in UV absorption. There is a loss of energy as concentration increased due to the inelastic scattering occurs in UV analysis. The phase transition occurs as we increased the different concentration of L- Phenyl Alanine. For one-mole and two-mole concentration crystal system is monoclinic and for five-mole concentration, the crystal system is orthorhombic. The particle size analyzed by Powder peak pattern of this crystals. The size and strain graph plot of William-Hall plot and crystalline size distribution graph of Warren-Aver Bach method interprets strain coefficient, size coefficient and L-graph of (Δd/d)% versus length of peaks pattern predicted by PXRD data.

Keywords: UV-Vis, FT-IR, PXRD, Williamson-Hall plot, Warren-Aver Bach method.

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DOI: https://dx.doi.org/10.5281/zenodo.1171297

Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials

Powder diffraction pattern analysis and FT-IR spectrum analysis of tetrakis(4-aminopyridine-kN^1)-di chloride copper(II) monohydrate crystal

M.Renugadevi**,** P.Jayanthi, P.Lalitha,S. Ilakkiyaselvi, S.Mohanraj,**A.Sinthiya***

PG & Research Department of Physics, SrimadAndavan Arts and Science College (Autonomous), Trichy-5. TamilNadu.

*Corresponding Author Email: sinthi@andavancollege.ac.in, Cell No: 9486732241

Abstract:

This paper Investigatesthe Tetrakis(4-aminopyridine-kN^1)-dichloridocopper(II) monohydrate crystals prepared by the slow evaporation method and characterized by Fourier Transform of Infrared analysis and Powder X-Ray diffraction techniques.We observed strong absorption bands occur in FT-IR and confirm the functional group. Thecrystal crystallized in triclinic system and particle size, systematic absences all changes analysed by powder peak pattern of this crystals. The Size and Strain graph plot of Williamson-Hall plot and crystalline size distribution graph of Warren-Aver Bach method interprets strain coefficient, size coefficient and L graph of (Δd/d) % versus length of peaks pattern predicted by PXRD data.

Keywords:Powder XRD, FT-IR, Williamson-Hall Plot, Warren-Aver Bach Method.

Reference

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DOI: https://dx.doi.org/10.5281/zenodo.1171301

Bulk superconductivity at $T_c = 0.79$ K in $Eu_2SrBi_2S_4F_4$: An AC-susceptibility investigation

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Abstract:

$Eu_2SrBi_2S_4F_4$ and $EuSr_2Bi_2S_4F_4$ have been synthesized [1] and investigated by recently designed a fully automated AC susceptometer for milli-kelvin temperature in Dynacool PPMS [2]. They are derivatives of the novel parent compound $Eu_3Bi_2S_4F_4$, [2] which shows superconductivity at 1.5 K [3] and is different from other BiS_2 superconductors in that it is an intrinsic superconductor; namely, no external doping is required to induce superconductivity (SC). As a result of Sr-substitution at the Eu-sites in $Eu_3Bi_2S_4F_4$, T_c was initially found to decrease from 1.5 K to 0.87 K for (x = 0.5) and then to 0.48 K in $Eu_2SrBi_2S_4F_4$ [3] and no sign of SC can be detected on further increasing Sr content at x=2 down to 0.3 K in $EuSr_2Bi_2S_4F_4$ [3]. Results of our new magnetic measurements show $T_c \sim 0.79$ K [4] in $Eu_2SrBi_2S_4F_4$ which represents a substantial enhancement in T_c as compared to $T_c = 0.48$ K reported earlier. This suggests an improvement of the quality of the sample. The decreased Eu^{3+} population resulting in corresponding decrease in charge carrier density, may be the main reason for the suppression of superconductivity [4]. Here we report [5] temperature dependence of the AC susceptibility $\chi_{ac}(T)$ of $Eu_2SrBi_2S_4F_4$ superconductor. AC susceptibility is measured with an AC drive field with frequency of 4125 Hz and amplitude of 0.02 Oe. The DC applied field was initially fixed at zero to check the superconducting transition temperature and then increased to 10 Oe and then goes up to 440 Oe to check the AC losses in the mixed state. Both the real (χ') and imaginary (χ'') parts of the AC susceptibility were measured. χ' shows a sharp diamagnetic transition at ∼0.79 K confirming the bulk superconductivity in $Eu_2SrBi_2S_4F_4$. On the other hand, χ'' exhibited a single, sharp, positive peak at around the same temperature. The presence of a single sharp peak in χ'' is indicative of better coupling of the superconducting grains in the studied $Eu_2SrBi_2S_4F_4$ superconductor. Further, under an applied DC field upto 440 Oe, the χ' diamagnetic transition shifts to a lower temperature 0.29 K, and the corresponding χ'' peak is broadened and shifted to the same lower temperature. This is usual for a type-II superconductor. At a DC field of 440 Oe, neither χ' nor χ'' showed transitions, which is indicative of rapid suppression of the superconductivity.

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DOI: https://dx.doi.org/10.5281/zenodo.1171375

Magneto-electric Coupling in $BaTiO_3/Sr_2CoO_3F$ heterostructure

Dr. Kartick Tarafder & Ramesh Reddy

ABSTRACT

By means of first-principles calculations, we study the electronic and magnetic properties of a cobalt oxyhalide[1] Sr_2CoO_3F (SCOF) perovskite in a hybrid heterostructure, combined with $BaTiO_3$ (BTO) in different polarization states (see Fig 1.). The calculations show that the spin state of Co atom in SCOF changed from High Spin (HS) state to Intermediate Spin (IS) state by introducing ferroelectric state in BTO. The IS state of SCOF system shows the half-metallic nature due to strong p-dσ hybridization[2]. The change in spin state of Co atom controlled by altering the polarization direction. Such changes in spin state results a large magneto-electric coupling constant. Moreover, this change in spin state by applying the polarization opens the possibilities to design and develop new type of future spintronic devices, in particular, storage devices by controlling the magnetism with electric fields.

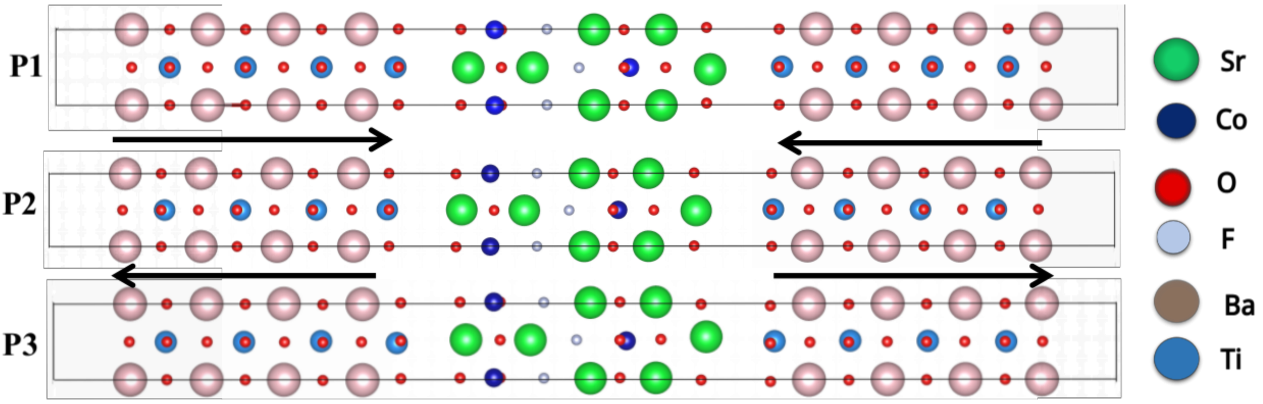

Fig 1: Atomic structure of of three types BTO-SCOF-BTO [001] multilayer configurations. P1 is Nonpolar system, BTO is paraelctric, P2 and P3 are polar systems, BTO is ferroelectric. The arrows mark the polarization orientation.

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DOI: https://dx.doi.org/10.5281/zenodo.1171389

Magnetic and Magnetocaloric properties of $Dy_6Ni_2Si_3$ compound

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Abstract

Systematic investigations were carried out on the magnetic and magnetocaloric properties of arc melted $Dy_6Ni_2Si_3$ compound.The polycrystalline compound shows two ferromagnetic (FM) transitionsat T_1 = 44 K and T_2 = 72 K respectively (Fig. 1). A slight spin reorientation like behavior is observed below T_1 around T= 26 K. The isothermal magnetization curve for T = 2 K reveals the presence spin reorientation at a critical field of 5 T. The magnetic entropy change (ΔS_m) computed from the isothermal magnetization data shows a maximum of 16.3 J/kg.K at 72 K for 9 T. Also, the presence of two magnetic transitions at T_1 = 44 K and T_2 = 72 K induces a table like magnetocaloric effect in a wide temperature range with a refrigerant capacity of 600 J/kg for a field change of 9 T. It also exhibits considerable negative magnetoresistance of 10% in 9 T at 2 K. Hence the magnetic properties observed for $Dy_6Ni_2Si_3$ are interesting for low temperature magnetic refrigeration. The detailed discussion on the magnetic properties will be presented in the symposium.

Keywords: Magnetocaloric effect, Spin reorientation, Magnetoresistance

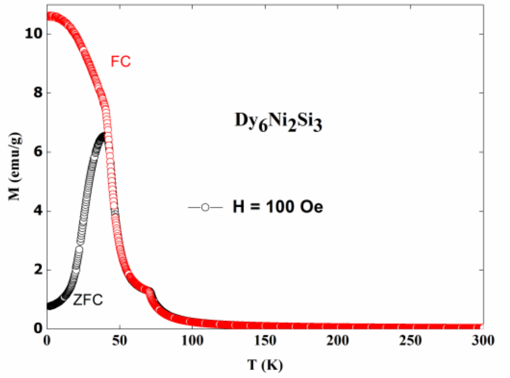

Fig. 1. Temperature dependence of ZFC and FC magnetizations at H = 100 Oe

DOI: https://dx.doi.org/10.5281/zenodo.1171393

Antimicrobial results of two different doping concentrations of CNT with ZnO

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Abstract

CNT is doped with Zinc source material of Zinc acetate by using hydrothermal synthesis. The prepared materials with two different proportions was analysed as XRD and SEM with EDAX using sophisticated instrument to confirm expected elements present with strong bond by evaluating and serious care on diffraction peaks which becomes sharper, surface morphology and energy dispersive amplitude. From the analysis of XRD, we found that all the crystal phases are anatase formation and there is a characteristic peak of ZnO at 2θ values which matches with JCPDS 36-1451 and JCPDS 26-1079 which is corresponding to CNT. TEM and SAED investigated the entitled compound that particles size, shape and presence of oxygen under Zn and CNT remand. The successful expected result has been obtained and explained after its serious analyzing antibacterial research stations that announcing the great attention for ability of bacterial inhibition.

Key words: ZnO-CNT, SEM, EDAX and Antibacterial.

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DOI: https://dx.doi.org/10.5281/zenodo.1171397

First principles study on Pd_2ZrGe full heusler alloy using density functional theory

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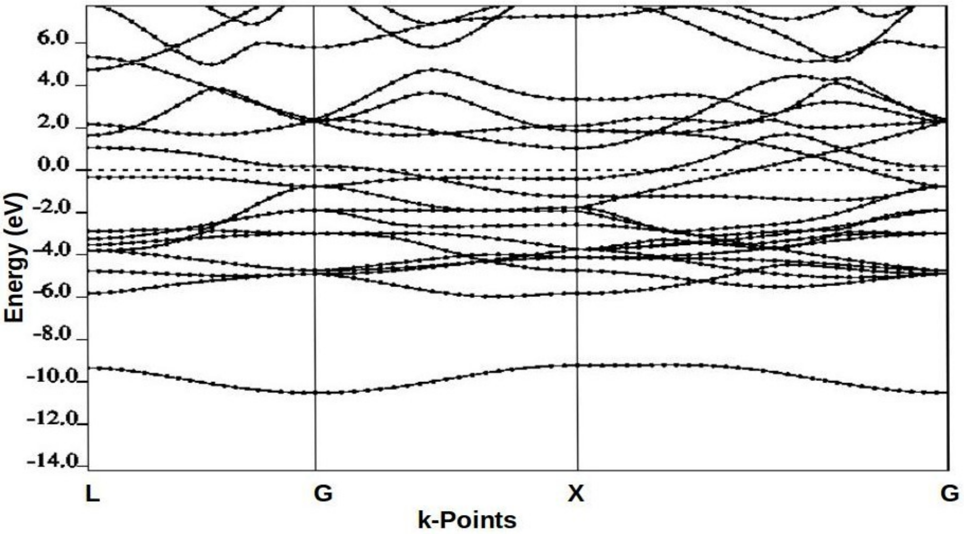
Abstract:

Electronic structure calculation using density functional theory was carried out for the hypothetical heusler alloy Pd_2ZrGe using PWscf code. The equilibrium lattice parameter was obtained by fitting the energy vs volume data to Murnaghan equation of state. Band structure, density of states and phonon frequencies were calculated for the optimized structure. The structure was optimized using BFGS method for both ionic and volume optimization. Band structure was calculated for both non magnetic and magnetic structure. Pseudopotentials which used for the calculation is GGA type which was generated using Troullier-Martins pseudization method.



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DOI: https://dx.doi.org/10.5281/zenodo.1171407

A study of magnetic phase transition in $BiFe_{0.5}Cr_{0.5}O_3$ thin films deposited over Pt (111)/Ti/SiO_2/Si substrate

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Abstract

$BiFe_{0.5}Cr_{0.5}O_3$ (BFCO) nanostructured thin films were prepared by sol-gel method over Pt (111)/Ti/SiO_2/Si substrate. The crystal structure of $BiFe_{0.5}Cr_{0.5}O_3$ films has been investigated using X-ray diffraction and it reveals that the films are formed at a high crystalinity with high degree of orientation depending on the deposition conditions. Rietveld refinement for the film has been done using Jana 2006. The multiferroic character of BFCO is proven by ferroelectric and magnetic measurements showing that the films exhibit both ferroelectric and magnetic hysteresis at normal room temperature. In addition, Spin-cooling behaviors of BFCO films have investigated through temperature dependent magnetic studies from 0 K to 300 K.

Keywords: Multiferroic, refinement, spin-cooling

DOI: https://dx.doi.org/10.5281/zenodo.1171409

An effective conventional powder metallurgy route using elemental powders for the development of Cu-Al-Ni shape memory alloys

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During recent years, Cu-based Shape Memory Alloys (SMAs) are in great demand due to their potential use as sensors, actuators and damping devices. In particular, Cu-Al-Ni alloys possess high thermal stability at elevated temperatures, i.e., above 373 K, making them suitable for high temperature. The preparation of these alloys through casting route results in a coarse-grained structure, which further coarsened during subsequent heat treatment. As a result, the mechanical properties especially ductility of the alloy becomes relatively poor due to brittleness and limit their applications. It has been suggested that the powder metallurgy processing may be a better alternative to enhance the ductility of the SMAs as this processing route may lead to more stable fine grained structure. Initially, the mechanical alloying of the elemental powders in order to make a mechanically alloyed powder having the desired composition One of the most important features of the Cu–Al–Ni SMAs produced by the powder metallurgy route is that the products have finer grains as compared to those produced by the liquid metallurgy route. Further, requirement of long milling time & milling in inert atmosphere for mechanically alloyed powder are very expensive and energy inefficient. Moreover, mechanical alloying may cause introduction of impurities and unwanted secondary phases in the matrix. Therefore, it was felt necessary to develop a simple powder metallurgy process (mixing, compaction and sintering/hot pressing) which can provide Cu-based shape memory material with homogeneous and controlled composition possessing improved properties. Preparation of the mixture of elemental powders in required composition followed by thorough mixing in dry condition followed by controlled heating cycle with pressure assistance. The sintered samples were further solutionized followed by quenching. Further the study was performed to observe the effect of aluminum concentration on the microstructure and phase evolution of the Cu based SMA. The FE-SEM and XRD analysis indicate that complete formation of martensite occurred in all the cases. However, increasing aluminum concentration resulted in the formation of higher amount of γ' martensite.

Keywords: Powder metallurgy, Shape memory alloy, Cu-Al-Ni, martensite

DOI: https://dx.doi.org/10.5281/zenodo.1171413

Structural Changes in Lead Phosphate Glasses doped with Vanadyl

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A series of lead phosphate glass doped with vanadyl were prepared by a single -step process from PbO and $NH_4H_2PO_4$. In these glasses the transition metal ion as vanadyl VO^{2+} ion derived from $VOSO_45H_2O$ as VO^{2+} (VS) doped and VO^{2+}(VP) is used as another dopant derived from V_2O_5. A thorough Knowledge of optical properties of transparent glasses will enable successful utilization of glasses for optical applications such as windows, filters and lasers. The optical absorption spectra of these glasses in the ultra-violet region have been recorded. The results obtained on the electronic absorption spectra observed to d-d bands. The VO^{2+} ions along with the double-bonded oxygen exist in a molecular complex which is identified as VO_5 polyhedra in lead phosphate glass network. As the Pbo content in the glass increases, structural changes take place in the network. The IR Spectra of these glasses were also presented with the results.

Keywords: 1. VANADYL 2. VO_5 polyhedra 3.d-d bands 4. VO^{2+} (VP) 5. VO^{2+} (VS)

DOI: https://dx.doi.org/10.5281/zenodo.1171472

Facile fabrication of SnS and activated carbon nanocomposite for the simultaneous determination of uric acid, theophylline and caffeine

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Abstract

Metal sulfide nanostructures offer particular advantages to electrocatalytic performance due to their large specific surface area and easy transport of analyte. Tin sulfide (SnS), one of the important metal sulfides possess orthorhombic layered crystal structure and have a direct bandgap of about 1.32-1.5 eV, has been extensively used for electrocatalyst, lithium ion batteries, dye-sensitized solar cells *etc.* due to their high electronic conduction, low cost, nontoxicity, easy of production and storage (1). In recent years, metal sulfide-carbon composite materials have attracted a great deal of attention due to their improved electrocatalytic properties. Here, we have adopted an attractive strategy to develop SnS/activated carbon (SnS/AC) composite nanostructures, where the carbon system ensures improved electrical contact between SnS nanoparticles.

Novel activated carbon (AC) materials were prepared from the ridge gourd luffa *(Luffa acutangula)* by an eco-friendly method. Tin sulfide -activated carbon composite (SnS/AC) was synthesized by a facile one-step hydrothermal approach. The prepared nanocomposite was characterized by XRD, FTIR, FE-SEM and Raman spectroscopy. Further, the SnS/AC composite has been used for the electrochemical simultaneous determination of uric acid (UA), theophylline (TP) and caffeine (CAF). The SnS/AC modified GCE showed an excellent electrocatalytic activity for resolving the overlapping voltammetric responses of UA, TP and CAF into three well-defined voltammetric peaks. The fabricated sensor responded to UA, TP and CAF over a wide concentration range with lowest detection limit. It has an excellent anti-interference ability against electroactive species and metal ions and proved to be useful to estimate UA, TP and CAF content in the urine and energy drinks with satisfactory recovery.

Keywords: *SnS, Activated carbon, uric acid, theophylline and caffeine, biosensors*.

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DOI: https://dx.doi.org/10.5281/zenodo.1171474

Bimetallic nanoparticles anchored on α-Fe_2O_3 catalyst for simultaneous electrochemical detection of dopamine and uric acid

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Abstract

We have found that magnetic α-Fe_2O_3 nanocubes exhibit an intrinsic catalytic activity toward the electrochemical sensing of dopamine (DA) and uric acid (UA). Au–Pd bimetallic nanoparticles, which act as efficient signal amplifiers, can be attached to the surface of α-Fe_2O_3 particles to further enhance the catalytic electrochemical signals. The one-step synthesized α-Fe_2O_3 @Au–Pd hybrid nanostructure shows significantly well-separated oxidation peaks with enhanced peak currents of DA and UA. We then demonstrated the use of this nonenzymatic nanoelectrocatalyst for individual detection, and the linear responses of DA and UA were in the concentration ranges of 100 nM $^{-1}$ mM and 1 µM $^{-1}$ mM with detection limits of 1.34 X 10 $^{-10}$ M and 1.8 X 10 $^{-6}$ M (S/N = 3σ/b), respectively. For simultaneous detection, the same detection ranges were retained with significantly lower detection limits of 1.38 X 10 $^{-11}$ M and 597 nM, respectively. The fabricated sensor was finally applied in selectivity tests for the detection of DA and UA with satisfactory results. The practical analytical utility was illustrated by selective measurements of human urine, serum and pharmaceutical drugs without any preliminary treatment.

Keywords: *α-Fe_2O_3 nanocubes, Au–Pd bimetallic nanoparticles, dopamine, uric acid.*

DOI: https://dx.doi.org/10.5281/zenodo.1171494

DNA mediated electrocatalytic enhancement on α-Fe_2O_3-PEDOT-C-MoS_2 hybrid nanostructures for Riboflavin detection on Screen Printed Electrode

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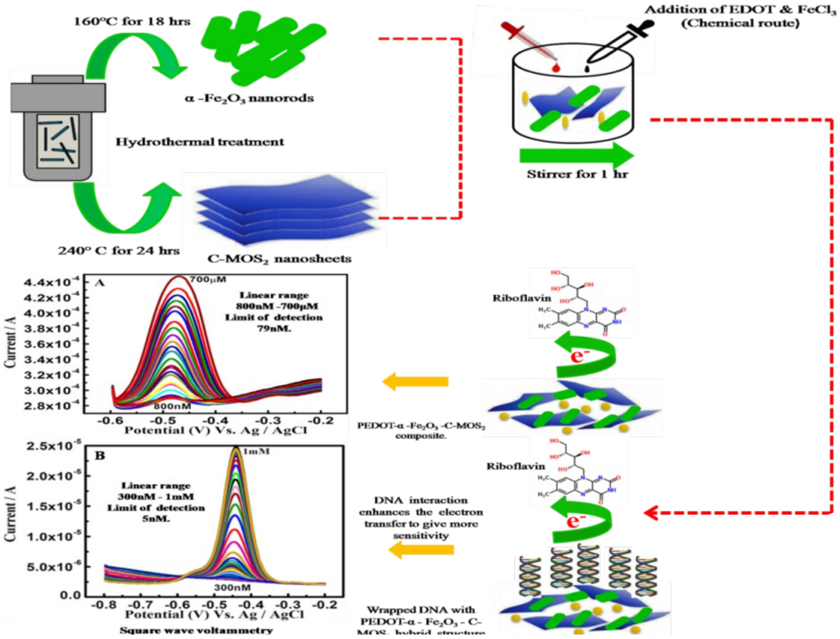
Abstract

Facile synthesis of iron oxide nanorods and PEDOT(poly(3,4-ethylenedioxythiophene) nanospheres on carbon supported MoS_2 (C-MoS_2) is reported for riboflavin (RF) sensing. Further, a novel aqueous-based DNA wrapped up with α-Fe_2O_3-PEDOT-C-MoS_2 scaffold shows high electrocatalytic activity compared to that of α-Fe_2O_3-PEDOT-C-MoS_2 composite in biosensing. The α-Fe_2O_3-PEDOT-C-MoS_2/GCE demonstrates the linear response of RF in the concentration range of 800 nM–700 µM, with detection limit 79 nM (S/N=3σ/b) whereas α-Fe_2O_3-PEDOT-C-MoS_2-DNA/GCE composite shows a wider range 300 nM–1 mM, with low detection limit 5 nM comparatively. Similarly, α-Fe_2O_3-PEDOT-C-MoS_2-DNA/SPE exhibits still wider range of 100 nM–1 mM, with detection limit 12 nM. Interestingly, it is also observed that the α-Fe_2O_3-PEDOT-C-MoS_2-DNA/GCE reduces the oxidation potential of RF by 30 mV. Thus the excellent behavior of proposed biosensor can be attributed to the unique behavior of DNA in giving wider detection range and good electrocatalytic behavior towards RF. The fabricated sensor exhibited highly sensitive and selective detection of RF. The real sample analysis was also executed in human urine, milk powder and pharmaceutical drug without any preliminary treatment.

DOI: https://dx.doi.org/10.5281/zenodo.1171536



DOI: https://dx.doi.org/10.5281/zenodo.1171536

Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials

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MOLECULAR STRUCTURE, NMR, HOMO-LUMO AND VIBRATIONAL ANALYSIS OF GAMMA O- NITROBENZALDEHYDE OXIME BASED ON DENSITY FUNCTIONAL THEORY CALCULATIONS

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ABSTRACT

In this work, the experimental and theoretical spectra of O- Ntrobenzaldehyde oxime were studied. The FTIR and FT-Raman spectra of O- Ntrobenzaldehyde oxime have been recorded in the region 4000-400 cm^{-1} and 4000-50 cm^{-1}, respectively. The molecular structure, geometry optimization and harmonic vibrational frequencies have been investigated. The spectra were interpreted with the aid of normal coordinate analysis based on the density functional theory (DFT) using the standard B3LYP/6-31G* method and basis set combination and was scaled using multiple scale factors yield good agreement between observed and calculated frequencies. The results of the calculations are applied to simulate Infrared and Raman spectra of the title compound which showed reasonable agreement with the observed spectra. The substituent of nitro group which is electron withdrawing group in an aromatic ring system makes a remarkable effect on the geometric and spectroscopic properties of the title compound are also discussed. Quantum chemical parameters such as highest occupied molecular orbital energy (E_{HOMO}), the lowest unoccupied molecular orbital energy (E_{LUMO}), energy gap (ΔE), chemical potential (P_i), global hardness (η), and the softness (σ) were calculated. ^{1}H and ^{13}C nuclear magnetic resonance (NMR) chemical shifts of the molecule were calculated by using gauge invariant atomic orbital (GIAO) method. In addition, molecular electrostatic potential (MEP) and Mulliken atomic charges were determined. Thermodynamic properties of the title compound have been calculated.

Key words: O- Ntrobenzaldehyde oxime, Vibrational frequencies, HOMO-LUMO, NMR.

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DOI: https://dx.doi.org/10.5281/zenodo.1171564

THERMO ACOUSTICAL INVESTIGATIONS OF MOLECULAR INTERACTIONS IN ANTIBIOTIC NORFLOXACIN

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ABSTRACT

A investigation of possible molecular interaction of antibiotic Norfloxacin is carried out to provide insight of molecular orbital (or) other calculation designed to elucidate electronic and conformational aspects of molecule are now used based on certain physical and bio-chemical properties. This is carried out through ultrasonic investigations at temperature 303K.

The ultrasonic velocity, density and co-efficient of viscosity were measured and the thermo acoustical parameters like adiabatic compressibility, acoustics Impedance, intermolecular free length and internal pressure were derived and these parameters describes the molecular interaction of aqueous Norfloxacin particularly the hydrogen bonding with the structural change of water molecules.

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DOI: https://dx.doi.org/10.5281/zenodo.1171596

Characterization of Al-6061 based metal matrix composite fabricated by stir casting route and modified by friction stir processing (FSP)

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Abstract

As 6061 Al-alloy possess high strength to weight ratio and having good corrosion resistance, it is used for automobile parts although having this advantage it has poor wear resistance which limits its application however metal matrix composite (MMC) in which hard ceramic particle such as SiC is dispersed leads to good improvement in wear and stiffness but in expense of ductility moreover uniform dispersion is very difficult in stir casting route so Friction stir processing (FSP) is done afterward since FSP is a novel technique and can be used for surface modification in composites by microstructure refinement and mechanical property enhancement. In this work Study has been carried out to explain the effect of FSP on the Al-6061/SiC_p (MMC) which is fabricated by stir casting technique, Aluminium matrix composites (AMCs) reinforced with 2% vol. SiC particle of size (20-160) µm which was then hot rolled at 420°C to minimize casting defects such as porosity later on modified by FSP. FSP has been conducted with 750, 1525 rpm of tool speed having cylindrical pin profile and keeping other variables such as traverse speed (50mm/min), tool geometry to be constant. In the present work the comparison of properties between cast Al-6061 alloy, SiC reinforced AMC (without FSP) and SiC reinforced AMC (with FSP) has been carried out. Microstructure, wear property, tensile properties and Vickers hardness test were investigated and characterization of the composite is done using X-ray diffraction, optical and scanning electron microscopy. X-ray diffraction patterns of Al-6061/SiC_p AMCs revealed the presence of SiC particles without formation of any other intermetallic compounds. Primary results showed more homogeneous distribution of SiC_p in FSP zone than base metal and an improvement in mechanical properties which is due to grain refinement. Significant improvement in the ductility was observed after FSP when compared with cast composite.

Keywords : FSP, Nanocomposites, 6061 Al-alloy

DOI: https://dx.doi.org/10.5281/zenodo.1171618

Ferromagnetic cluster spin glass nature in $Sm_3Ag_{2.55}Al_{8.45}$

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Abstract

Spin glass (SG) has become one of the main streams of research in condensed matter physics over the years [1-2]. However the real origin of this behaviour is still under debate. The compound $Sm_3Ag_{2.55}Al_{8.45}$ is reported to adopt the orthorhombic La_3Al_{11} structure type. The indication for the presence of ferromagnetic SG was obtained from the anomalous behaviour in ac susceptibility besides ferromagnetic ground state in dc susceptibility. Susceptibility exhibits a slope change at T_C =15 K. The irreversibility between zero field cooled (ZFC) and field cooled (FC) is highly dominant below the freezing temperature T_f = 13.3 K, 11 K, 9 K, 5 K for the steady fields of H = 100 Oe, 1 kOe, 3 kOe, 10 kOe respectively. The non- vanishing of irreversibility in magnetization for an applied field of H= 20 kOe, which is relatively large for FM materials suggests the presence of randomly quenched ferromagnetic clusters below T_C =15 K [3, 5]. In this symposium, a detailed discussions will be presented on the structural, ac and dc magnetic susceptibility, isothermal magnetization, and heat capacity investigations on a polycrystalline $Sm_3Ag_{2.55}Al_{8.45}$ sample which exhibits ferromagnetic spin glass behaviour.

Keywords: Spin glass, ferromagnetic, heat capacity

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DOI: https://dx.doi.org/10.5281/zenodo.1171644

Growth, Vibrational, Optical, Mechanical and Dielectrical studies of EDTA Doped Cupric Sulphate-Zinc Chloride Crystals

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Abstract

The Zn is a conventional semiconducting material, whereas Cu is a common metal, and both are having the centro-symmetry structure independently. The Ethylene Diamine Tetra Acetic acid (EDTA) is a hexa dentate ligand, and it binds with central metal ions through the four oxygen and two nitrogen atoms [1]. Hence, the doping of EDTA with Zn and Cu individually can provide NLO property to these elements. Here, crystals of Ethylene Diamine Tetra Acetic acid (EDTA) doped Cupric Sulphate Zinc chloride (Cu-Zn) was grown by Slow Evaporation Solution Technique from an aqueous solution. Powder X-ray diffraction was performed to assess the crystalline nature. Structural analysis by the functional groups was investigated using FT-IR spectroscopy, and the shifting of frequency represents the coordination of EDTA in the grown crystal [2]. Fluorescence Spectra was recorded to explore its emission properties. Mechanical behavior was analyzed using the Vickers microhardness test. The variation of microhardness number with applied load explains the RISE behavior of the grown crystal. Using Wooster's empirical relation the elastic stiffness constant (C_{11}) was calculated from the Vickers hardness values at different loads. The impedance analysis was performed to characterize the electrical properties as a function of frequency to understand their relaxation and conduction mechanism. These studies were confirmed the enhancement of all these physical properties of Cu-Zn by doping of EDTA.

Keywords: Crystal growth, SEST, Powder XRD, FTIR, Mechanical strength.

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DOI: https://dx.doi.org/10.5281/zenodo.1171688

Study of Vibrational, Mechanical and Dielectrical Properties of ADP Single Crystal

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Abstract

Several research works have been carried out on pure and doped ADP crystals, because of its unique non-linear optical, dielectric, antiferroelectric and piezoelectric properties [1]. Moreover, it was the first material that were used and exploited for their non-linear optical and electro-optic properties [2]. Here, With an aim of finding new useful materials for academic and industrial use, an attempt has been made to grow the single crystals of ADP using the salt water as solvent. The crystalline nature and various planes of reflections were studied using Powder X-ray diffraction analysis. The Presence of functional groups in the grown crystal was identified using Fourier Transform Infrared Spectroscopy. Vicker's microhardness test was employed to study the mechanical strength of the grown crystal. The variation of Vickers hardness with applied load indicates that the crystal exhibit Reverse Indentation Size Effect (RISE). The grown crystal has soft nature confirmed from Meyer's law. Dielectric properties such as dielectric constant and dielectric loss were studied as function of frequency for varying temperature. The low dielectric loss at higher frequency implies that grown crystal has good optical quality and lesser defects.

Keywords: ADP, RISE, Dielectric property, mechanical strength.

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DOI: https://dx.doi.org/10.5281/zenodo.1171697

Room Temperature Ferromagnetism in Group I Elements Codoped ZnO:Mn Nanomaterials

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Abstract

ZnO is a wide bang gap II–VI semiconductor known for its multifunctional properties and interesting applications in the field of magneto-electrics and magneto-optic devices [1]. ZnO based DMS materials have been attracting much interest of potential spintronics devices such as spin-valve transistors, spin light emitting diodes, and non-volatile storage [2]. Dietl et al. predicted theoretically the room temperature ferromagnetism (RTFM) behavior in Mn doped ZnO [3]. In this present work, we report that the structural, optical and magnetic behaviour of monovalent group I elements (Li^+ Na^+ K^+) codoped ZnO:Mn nanoparticles (NPs). The Mn doped and Group I elements codoped ZnO:Mn nanoparticles were prepared by co-precipitation method. The single crystalline phase formation of prepared NPs was confirmed by XRD and Raman spectroscopic technique. The presence of lattice defects was identified from the Raman and EPR spectral analysis. The room temperature ferromagnetic behaviour of prepared NPs was observed from VSM analysis. The presence of lattice defects induced ferromagnetism in prepared NPs. The observes results are discussed and reported.

Keywords: Nanoparticles, Room Temperature Ferromagnetism, Effect of Lattice Defects

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DOI: https://dx.doi.org/10.5281/zenodo.1171701

Atomic Layer Deposition - an Enabling and Critical Thin Film Technology

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Atomic Layer Deposition (ALD) is the most advanced thin film deposition technique that offers sub-nanometer precision. Originally invented almost half a century ago, and hereto neglected, ALD was brought up to forefront due to shrinking dimensions in chip manufacturing. ALD is a cyclic process and it is based on the principle of chemisorption which is self-limiting in nature. In an ALD process, substrate surface and gaseous chemical precursor interaction is of utmost importance. The substrate surface must have receptor chemical groups on it on to which the incoming gaseous precursor groups can lock on to like a lock and key. A typical ALD cycle comprises four pulses that are repeated to build the desired film thickness as shown in Fig. 1 below.

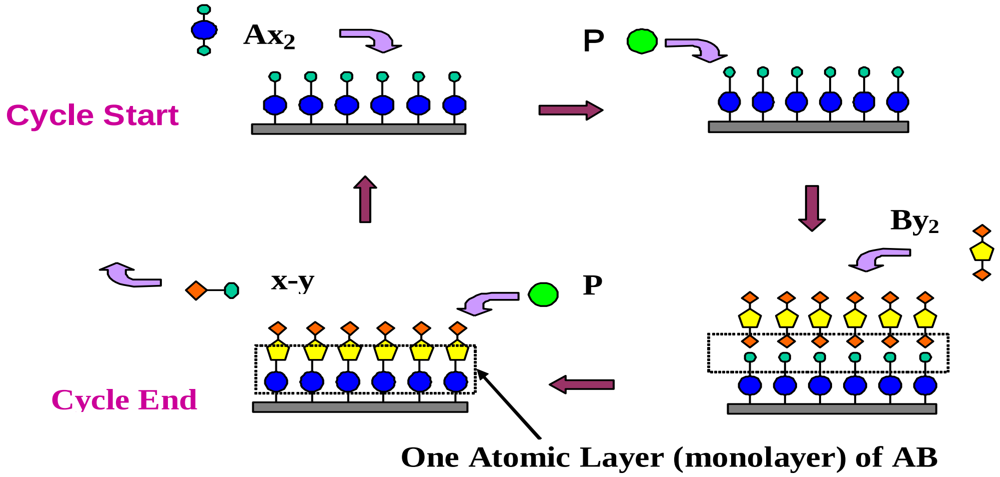
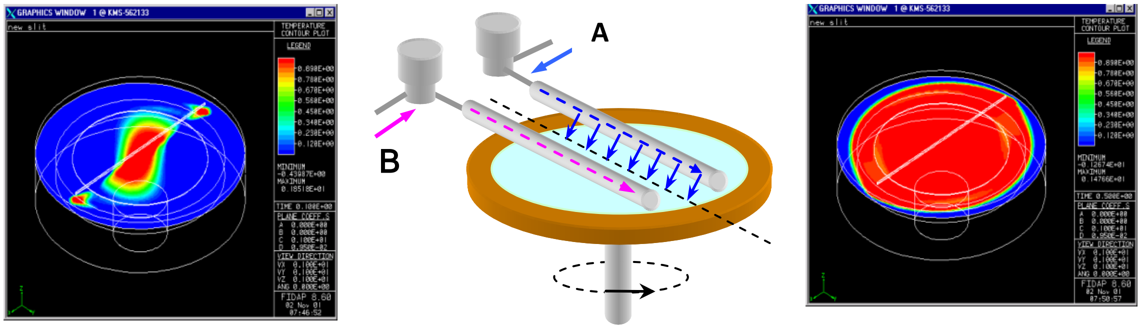


Fig. 1: Schematic representation of a cyclic ALD process. P is an inert gas pulse that drives away excess (physio-sorbed) or loosely attached precursor molecules from the surface thus forming a chemisorbed monolayer. This is the basis of an ALD reaction.

ALD offers extremely critical advantages unmatched by any other process at quite low cost: (a) precise, digital control of thin film thickness (b) large area deposition (c) fully conformal deposition over complex shapes and geometries at deep sub-micron level (d) very low defect and pinhole density (e) superior adhesion and (f) variety of materials – semiconductors, insulators, and metals. Thin film materials and their proven ALD processes are summarized by Suntola (ref. 1). Examples of thin film materials deposited by ALD are numerous. Among those: Si, GaAs, GaN, InGaN, ZnS/ZnSe, SiO_2, AlN, Al_2O_3, Cu, Ta, W, WN_x, TaN, TiN, TiO_2 and so on for fabrication of advanced silicon and optoelectronic devices, fuel cells, catalysts, flat panel displays.

The ALD process does not demand uniform spread of gaseous precursor nor does it require precise temperature uniformity of the substrate surface. An ALD chamber design is thus rather simple. However, this fact combined with the self- limiting nature of chemical process leads to ALD lower deposition rate ~ 1 nm/min. To remedy the situation, a novel ALD/CVD hybrid reactor design is devised as shown in Fig. 2 (ref. 2).

DOI: https://dx.doi.org/10.5281/zenodo.1171703



Surface coverage, t = 50 ms

Surface coverage, t = 500 ms

Fig. 2: Results of real-time computational fluid dynamics (CFD) simulation of the novel hybrid ALD/CVD reactor. Substrate T = 500 deg., at 60 rpm, 50 and sccm He flow.

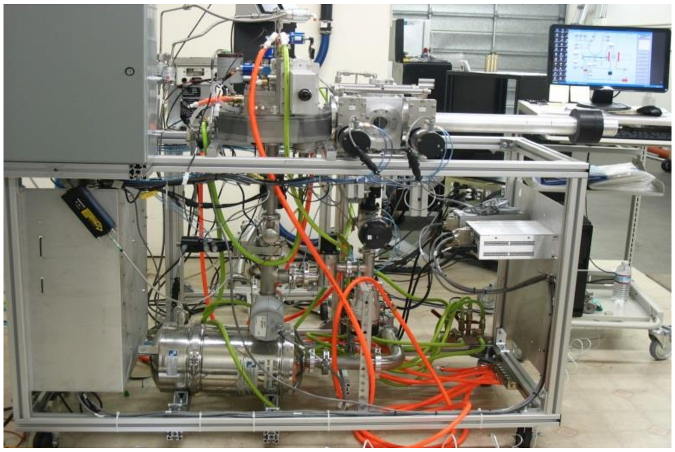


Fig. 3 (left) shows pictorial view of an ALD/CVD system developed by Atomic Precision with a manual wafer loading mechanism to deposit GaN thin films at low temperatures (below 500 °C) by employing N_2+ H_2 gaseous mixture in a linear pulsed microwave plasma (refer to Fig. 1, $By_2 = NH_x$ and $Ax_2 = GaCl_3$) to deposit GaN thin films for LED device fabrication. (ref. 3)

An advanced ALD reactor design concept called Turbo –ALD is shown schematically in Fig. 4 which can be useful to deposit large area (m^2) thin films on flexible substrates at 15 – 20 x speed than current systems (ref. 4)

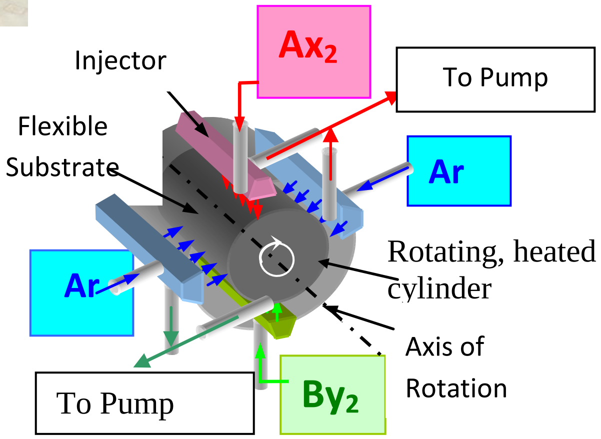


Fig. 4: Schematic of a Turbo-ALD reactor configuration.

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DOI: https://dx.doi.org/10.5281/zenodo.1171703

Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials

Kinetic analyses of thermogravimetric data of solid PCS up to 1673K in flowing Nitrogen

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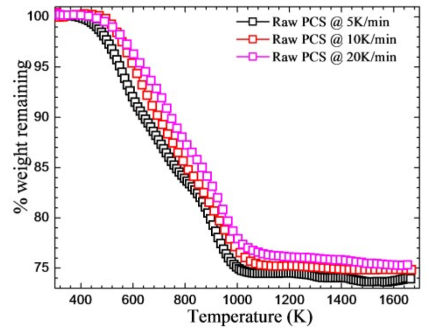
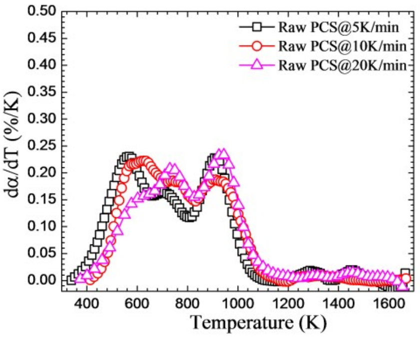
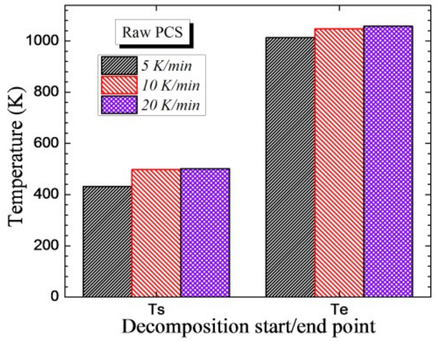
Abstract

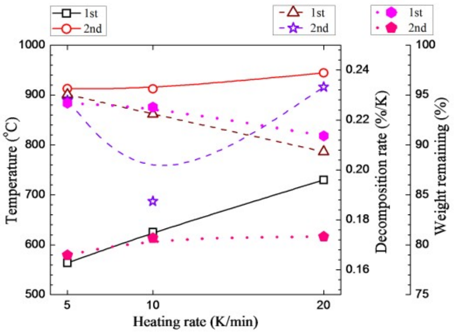
Pyrolysis kinetics of an indigenously developed solid PCS, a promising source of making SiC foams, have been investigated using TGA up to 1673K in N_2. Tests were performed at 5, 10 and 20K/min to assess the dependence of pyrolysis on heating rate. Primary decomposition of PCS was spanned over 430–1060K and the range shifted towards higher side at increased heating rate. On contrary, irrespective of heating rate, the PCS traced two distinct peaks in the DTG curves. While, the moderately low temperature peak (<750K) indicated loss of oligomars and water, the high temperature peak (≤950K) indicated loss of organic side groups and formation of inorganic state. To evaluate the *Arrhenius* parameters (E_a and A) of PCS pyrolysis, Coats-Redfern model was used. Comparatively slower reaction rate at low temperature regime with lower E_a (~50 kJ/mol) and higher rate during the second stage of pyrolysis having higher E_a (~120 kJ/mol) were obtained.

Key words: Polycarbosilane, TGA, Pyrolysis kinetics









DOI: https://dx.doi.org/10.5281/zenodo.1171709

Undoped and Mg^{2+}- doped TiO_2nanoparticelsfor DSSCs activity

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Investigates the influence of Mg^{2+}-doping on the dye-sensitized solar cells(DSSCs) behaviour of anatase TiO_2 nanoparticles. The undoped and Mg^{2+}-doped (1,3,5, and 7 at.%) TiO_2 nanoparticles are synthesized by sol-gel method. The effects of Mg^{2+}-doping on the structural and optical response of the prepared samples are investigated. XRD measurements are carried out to understand the structural properties of the synthesized samples. Transmission electron microscopy (HRTEM), and selected area electron diffraction (SAED) patterns are used to study their morphologies, particles size, crystallinity and lattice arrangements. The magnetic result demonstrated the prepared Mg^{2+}-doped TiO_2 nanoparticles exhibit room temperature paramagnetism.PL was carried out to study the defects in the samples. The presence of defect and their impact on the performance of DSSCs are demonstrated from the PL studies. Further, the current-voltage (I-V) measurements are done for the DSSCsfabricated from the synthesized photoanodes.

DOI: https://dx.doi.org/10.5281/zenodo.1171717

Thermoelectric behavior of ZnTe materials and its characterization

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Abstract

Zinc acetate source materials and tellurium oxide are the main sources to synthesize the ZnTe Nanoparticles. By hydrothermal synthesis, zinc telluride nanoparticles are prepared and characterized by using X-ray diffractrometer, Photo Luminescence Spectroscopy and Photo acoustics Spectroscopy. XRD analysis gave the result of crystal size lies within the range of 52 nm. This synthesized nano material was annealed to two different temperatures of 200^0C and 400^0C. For the annealed samples, crystal size increases to the values of 57nm and 63nm. The Ultraviolet Spectroscopy studies inferred that its absorption and bandgap values decreased and the crystal size increases. Photoacoustics spectroscopy gave the result of thermoelectric behavior of the samples. Thermal conductivity and Thermal diffusivity of the samples were calculated by using this technique.

Keywords: Zinc acetate, tellurium oxide, XRD, bandgap

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DOI: https://dx.doi.org/10.5281/zenodo.1171725

Fe_2O_3 thin films on deposited on ITO substrate and its RBS characterization

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Abstract

Fe_2O_3 thin film was deposited on the ITO plate by using Thermal evaporation technique. X-ray diffraction (XRD), Rutherford back scattering (RBS), and optical bandgap (BG) of the ITO in Fe_2O_3 system were studied. The optical and structural characteristics of the films were measured. The overall features of these XRD curves confirm the crystalline nature of the present samples and calculated the crystal size of the value nearly 43 nm. The UV-Vis study the band gap of Fe_2O_3 is 3.21 eV. Morphology of Fe_2O_3 presents which gives the better results are taken by AFM. Wave number 1407 cm^{-1} has the frequency vibrations of Fe_2O_3 samples. Fe_2O_3 and their concentrations ratio which affect the particles average size, thermal evaporation technique gives the different magnetic properties of the deposited sample. Though there is no hysteresis in the experimental curve, the discrepancy between the measured and calculated curves is observed that can be due to a wide distribution of particles size. The hardness and mechanical strength of the particle was analysed.

Keywords; Samarium, Thermal evaporation technique, SEM, AFM and RBS

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DOI: https://dx.doi.org/10.5281/zenodo.1171737

Synthesis and optical characterization of Yittrium doped Cerium Oxide Nanoparticles

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Abstract

In bio synthesis, boiling method is used to prepare Yittrium doped Cerium Oxide nanoparticles. Dates syrup (10 ml), Neem leaves extract of 10 ml was added to prepare this nanoparticles. Neem leaves extract and dates syrup which are acting as a reducing agent of Cerium Nitrate source material. Bio synthesized Yittrium doped Cerium Oxide was characterized by using X-Ray Diffractometer to confirm crystalline nature and structure of the nanoparticles. Scanning Electron Microscopy and Elemental X-Ray analysis was carried out to confirm the presence of metals in the nanoparticles. Magnetic studies explained the intensity of magnetization of the sample (emu/g) and coercivity of the sample. These magnetic studies were analysed by using Vibrating Sample Magnetometer. Bio activity of the samples were analysed from the studies of Anti bacterial and Anti fungal.

Keywords: Bio synthesis, Neem leaves, XRD, Anti bacterial, Antifungal

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DOI: https://dx.doi.org/10.5281/zenodo.1171743

Visible Light Photocatalytic Activity of ZnO-TiO_2Composites for the Degradation of Rhodamine B

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Abstract

High quality ZnO doped Titanium dioxide nanoplatelets were synthesized by hydrothermal method. Titanium dioxide plays an important role in Solar cells applications. Due to absorb the low-energy radiation, it tunes the optical property of Titanium dioxide. Composition, structure and morphology of the samples were analyzed .Characterization studies were done by X-ray diffraction and it clearly confirm the hexagonal wurtzite structure with same lattice constants; a=3.248Å and c=5.212 Å. It reveals the doped samples are improved without affecting the parent lattice. The morphological and optical properties of Zinc and Titanium oxide materials were studied by Scanning electron microscopy (SEM) and UV-vis spectroscopy. The Photocatalytic degradation of Rhodamine B dye under visible light radiation were studied by using different experimental condition in initial dye concentration and rate constant was calculated using L-H model.

Keywords: Composite materials, Colloidal processing, TiO_2 and ZnO

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DOI: https://dx.doi.org/10.5281/zenodo.1171745

Co doped SnO_2 nanoparticles for hydrogen gas sensing applications

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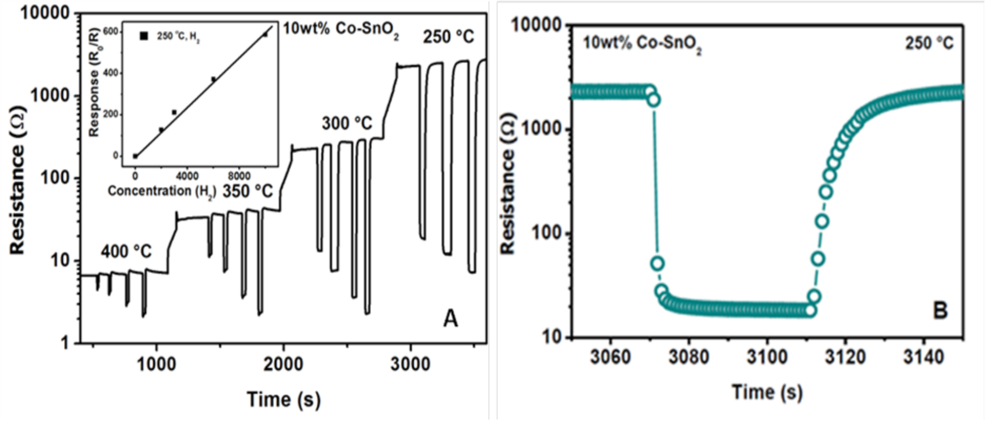
The recent advances in the materials science and nanotechnology enabled the development of smart sensors that can detect even very low level concentrations of analyte with high precision. SnO_2 has been extensively used as sensing material for the development and technological implementation of gas sensor and biosensor for various applications. Here, we report that the gas sensing properties of nanostructured SnO_2 could be improved significantly by suitably modifying its properties through various chemical (doping, composite formation, surfactant mediated synthesis) and physical (gamma ray, heavy ion irradiation) approaches.

Hydrogen is a highly flammable gas and will burn at concentrations as low as 4% in. Hence, the hydrogen leak sensors are very much essential for various applications. Resistive sensors based on Mn & Co doped SnO_2 nanoparticles have been fabricated and its sensing performances towards the detection of hydrogen (H_2) were investigated. Results demonstrate that the Co (10 wt%) doping is more effective in enhancing the sensing performance of SnO_2 NPs when compared to pristine and Mn-doped SnO_2, allowing the fabrication of a hydrogen sensor with excellent response and reproducibility at the operating temperature of 250°C.The selectivity of the fabricated sensors against the potential interfering gas carbon monoxide (CO) was also investigated.



Key words: SnO_2 nanoparticles, chemical doping, gamma irradiation, Hydrogen, carbon monoxide.

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DOI: https://dx.doi.org/10.5281/zenodo.1171751

Synthesis of novel multicomponent refractory alloys consisting of Mo, Nb, Ta and W

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Abstract

Multicomponent alloys consisting of four or more elements are being studied extensively and this is currently an active field of materials research. Since the discovery of the equiatomic FeCrMnNiCo alloy in the ‘70s by the research group of Cantor [1], literally hundreds of compositions have been studied [2]. The interest in these systems is not just in advancing our knowledge of mateials, but also from the viewpoint of practical applications, since many multicomponent systems have been shown to possess outstanding mechanical properties, resistance to corrosion, etc. Several of these alloys have also been observed to have high configurational entropy

This presentation discusses the synthesis of refractory alloys containing Mo, Nb, Ta and W for use in demanding environments. Since these metals melt at high temperatures, it is difficult to synthesize them using conventional methods such as solid state reaction. We have adopted a microwave-assisted process, wherein the formation of the alloy and its consolidation are expected to take place simultaneously. Since the mechanism of heating materials in microwaves is different as compared to other techniques, the kinetics of formation are also different. Results from preliminary experiments will be presented and a comparison with other methods will also be made.

Keywords: multicomponent alloys, high entropy, microwave-assisted synthesis

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DOI: https://dx.doi.org/10.5281/zenodo.1171753

Electrochemical preparation of graphene quantum dots from wood charcoal as a peroxidase mimetic

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Abstract

Horseradish peroxidase (HRP) has been extensively used in enzyme linked sorbent assay (ELISA) based disease diagnosis. Like other natural enzymes, the expensive steps involved in the production of HRP along with its extreme environmental sensitivity, limits its potential applications. To overcome these challenges considerable efforts have been made to explore HRP activity of nanomaterials. In present study, we highlight electrochemical synthesis of nearly uniform size (~ 5 nm) of graphene quantum dots (E-GQDs) from wood charcoal and their further application as colorimetric detection of H_2O_2 and glucose. E-GQDs allowed a rapid and sensitive detection of glucose with a detection limit of 0.006 mM for dynamic response range of 0.01–0.6 mM. Study introduces a cheap and widely available raw material for the electrochemical synthesis of graphene quantum dots with commendable enzyme mimetic activity which may have a huge impact in developing calorimetric bioanalysis systems.

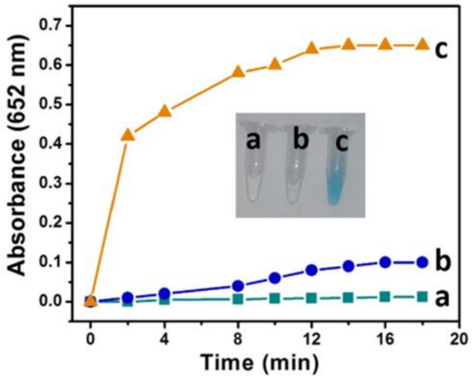

Figure: Time-dependent absorbance changes at 652 nm of TMB solution in different reaction systems

Keywords:**E-GQDs, Horse radish peroxidase (HRP), Glucose oxidase (GOx), Colorimetric, Peroxidase mimetic**

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DOI: https://dx.doi.org/10.5281/zenodo.1171758

Photocatalytic Graphene:TiO_2 Nanocomposites for Air Purification

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Abstract

Recently, Graphene and its composites are extensively explored by researchers for promising applications in the fields of energy, environment decontamination, energy storage, solar cells and photocatalyst [1-5] etc. The high electric charge carrier mobility , optical transparency, large surface area, easy chemical functionalization and mechanical strength with flexibility properties of graphene has made it as an ideal mechanical support, photo sensitizers and catalysts for nanocomposites development with enhanced performance depending upon the synergetic effects of components. In this work, graphene (G), TiO_2 nanoparticles (TN) and TiO_2 nanoparticles dispersed graphene nanocomposites (TG NC) have been prepared by chemical route for air purification. The structural, morphological, optical and vibrational properties of these powdered samples were characterized by using various analytical techniques to confirm their formation. The decontamination of polluted air by G, TN and TG NC reveals that TG NC is better than G and TN due to higher adsorptivity of contaminants and contaminant decomposition.

Keywords: Nanocomposite, graphene, TiO_2, Photocatalyst, Air Purification

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DOI: https://dx.doi.org/10.5281/zenodo.1171764

Density functional theory calculations for the enhanced quantum capacitance of chemically modified graphene nano-ribbon supercapacitor electrodes.

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Abstract

Graphene-based materials have been proposed as promising electrodes for super capacitors. Recently, it has been found that one of the limitations of graphene electrodes is the finite quantum capacitance. In this work, we investigate the impact of adatom adsorption or functionalization of graphene on the electronic structure and quantum capacitance. Density functional theory calculations were performed to simulate the electronic structure and the quantum capacitance variation with different adatom concentration. Chemical modifications with various width terminations of graphene nanoribbon are tried to enhance the quantum capacitance. We compared the quantum capacitance of graphene with different concentrations of oxygen on all possible positions. Our results clearly show that the number of oxygen containing groups and the location of oxide region largely influence the electronic properties of graphene nanoribbon and thus the quantum capacitance when compared to pristine graphene. Our work highlights the importance of the quantum capacitance in the overall performance of graphene-based super capacitors.

Graphene Nanoribbon , Chemical modification of GNR , Quantum capacitance.

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DOI: https://dx.doi.org/10.5281/zenodo.1171766

Nano-Au Particle Embedded Carbon Paste Electrode Sensing Platform for Electrochemical Detection of Temozolomide*in-vitro*

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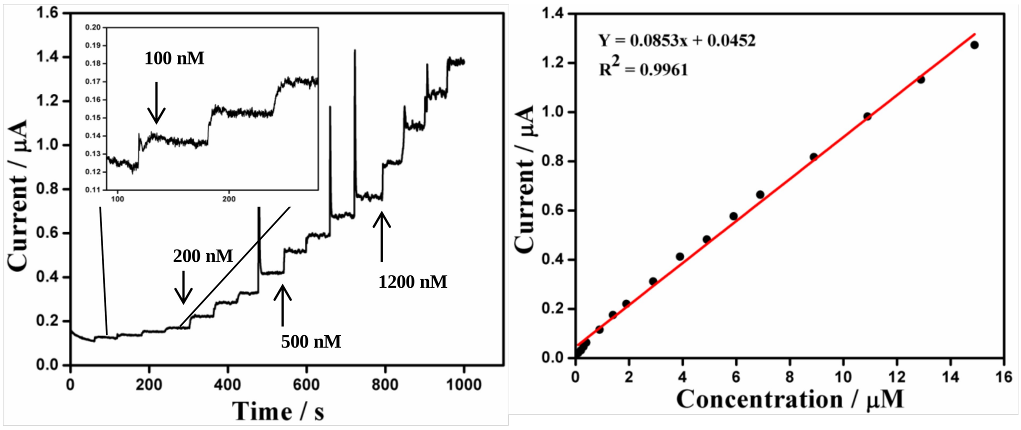
Abstract

A versatile reusable electrochemical biosensor system is proposed by using carbon paste electrode (CPE) embedded with gold nanoparticles for the detection an important antineoplastic alkylating agent Temozolomide (TMZ)[1]. A finite layer of nanogold is formed with the homogeneous distribution of gold nanoparticles bypotentiodynamicelectrodeposition technique. The surface of the fabricated sensor has been characterized by X-ray diffraction and FTIR for the structural and chemical properties of the sensor system. The electrochemical efficiency of the present sensor system towards the detection of TMZ has been evaluated by electrochemical impedance spectroscopy (ESI) and square wave voltammetry (SWV). Under optimized conditions, by applying SWV method, a linear calibration plot is achieved over the concentration range of 0.5 – 9 µM, and as low as 100 nM TMZ was determined in steady-state current-time analysis with the analysis time < 20 s.



Keywords: Electrochemical analysis, Antineoplastic agent, Nano-gold particles, Electrodeposition, Carbon paste electrodes.

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DOI: https://dx.doi.org/10.5281/zenodo.1171772

Tribo-mechanical behavior of spark plasma sintered multiwalled carbon nanotube reinforced AlN rich SiAlON polytype composites

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Abstract

Effect of MWCNT reinforcement on tribomechanical properties of SPS processed (2000°C/10 min/40 MPa) additive free, dense SiAlON polytype has been investigated. FESEM observation confirmed successful retention of CNT's tubular morphology with limited crumbling/shortening of defective CNTs after SPS processing. Besides formation of equiaxed and fibre-like SiAlON grains, different CNT/SiAlON interactions were also observed in the composite. Depending on test load, the 0.5 wt.% CNT/SiAlON composite offered 7.5–25% and 10–16% higher HV and K_{IC} values, respectively, over the monolith. Both sintered compositions showed positive *indentation size effect* and rising *R-curve* behaviour within the investigated loading range. More than 30% improvement in wear resistance was obtained for the composite compared to the pure polytype when scratched against a sharp diamond indenter under dry condition. Changes in tribomechanical properties of pure polytype through MWCNT reinforcement have been discussed with the help of microstructural and wear track features.

Key words: SiAlON polytype; MWCNT, SPS, Tribo-mechanical properties

DOI: https://dx.doi.org/10.5281/zenodo.1171780

Variation in tribo-mechanical properties of additive free SiAlON polytypoids densified under different SPS process temperature

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Abstract

The present work reports variations in tribomechanical properties of additive free SiAlON polytypoids as a function of spark plasma sintering temperature. While, at low sintering temperature (1600°C), the specimen was ~82% dense consisting of inadequately grown grains, sintering at 1900°C resulted in >98% dense polytypoid having fibre-like morphology. Irrespective of indentation load used, the 1900°C dense polytypoid offered ~4.5 times higher HV values over the 1600°C sintered specimen. The dense polytypoids offered HV as high as ~21 and ~16 GPa at 0.2 and 2 kgf, respectively. K_{IC} of the dense polytypoids under 10 kgf was found to be ~5.45 MPa-m$^{0.5}$ that indicated self-reinforcing effect offered by the needle shaped grains formed in the polytypoids. Unlubricated linear scratch tests revealed significant improvement in wear resistance at increased sintering temperature. Under 20N, wear rate and COF were found to be ~9.58 x 10^{-4} mm^3/N-m and ~0.35, respectively, for the 1900°C sintered specimen.

Key words: SiAlON polytype; SPS, Tribo-mechanical properties

DOI: https://dx.doi.org/10.5281/zenodo.1171782

Thermoelectric Performance of CdS QDs Based Hybrid Nanocomposites

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Abstract:

Thermoelectric (TE) materials can produce direct electrical power from a formed temperature gradient (1). They are extremely reliable, 'fuel-free' solid-state devices for energy generation. TE devices can play an important role in energy harvesting and energy efficiency, however, their development is limited due to lack of high efficiency achieved from the currently available materials. Recent developments based on nanomaterials have shown dramatic improvements (by a factor 2 to 3) in the performance of TE devices. In the present study, we have prepared CdS QDs based ternary hybrid nanocomposites (RGO/CdS/PANI, RGO/CdS/PEDOT: PSS) and studied their thermoelectric behaviour. The electrical conductivity, seebeck coefficient and power factor of these nanocomposites were calculated with various loading of RGO-CdS nanocomposite in both PANI and PEDOT: PSS. The final RGO-CdS-PANI nanocomposites delivered high electric conductivity and power factor. The effective band alignment and decreased thermal conductivity in RGO-CdS-PANI nanocomposite resulted in p-type behaviour and high zT value.

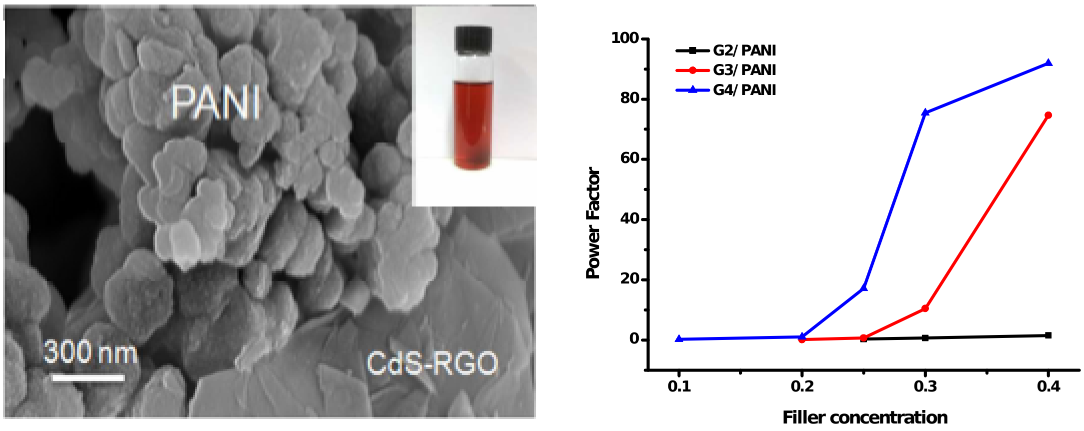

Fig. a) SEM image of RGO-CdS-PANI nanocomposite and inset photograph of its re-dispersion in ethanol b) Power Factor with filler concentration of RGO/CdS in RGO/CdS/PANI nanocomposite

Keywords: CdS quantum dots, Hybrid nanocomposites, Thermoelectric, Power factor.

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DOI: https://dx.doi.org/10.5281/zenodo.1171792

Giant exchange bias in $Zn_{0.3}Ni_{0.7}Fe_2O_4$ system

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Abstract

Exchange bias (eb) is an induced magnetic anisotropy.It is generally observed when ferromangnetic (FM/antiferromagnetic (AFM) interfaces are cooled through the Neel temperature (T_N) of the AFM component . These EB systems have promising applications in the field of magnetic recording, spin valves, permanent magnets etc .The hysteresis loop for an EB system when cooled through T_N in the presence of magnetic field, shifts along the field axis in the direction opposite to the cooling field (1-3). We have investigated the EB effects for Zn substituted Ni-ferrite with a specific compostion of $Zn_{0.3}Ni_{0.7}Fe_2O_4$. X-ray diffraction and transmission electron microscopy con fermed the phase-purity and particle size of the samples. Our principal aim was to observe EB by oberverving the interaction between the the surface and core of single-phase magnetic nanoparticles.

Exchange bias, magnetic anisotropy

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DOI: https://dx.doi.org/10.5281/zenodo.1171804

A detailed study of charge recombination dynamics in dye sensitized solar cells based on two triphenylamine based dyes

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Sustainable energy is going to be a more crucial problem than any other that we have. Solar energy is the most abundant and primary source of renewable energy that we can depend upon for our growing energy needs. Thus harvesting solar energy using photovoltaics has become a priority research area in physics and chemistry for the last several decades. Dye sensitized solar cells (DSSC) have emerged as a potential alternative to silicon based solar cells. Low production costs and environmental issues have prompted a search for metal-free organic sensitizers as alternatives for polypyridyl ruthenium(II) derivatives. Understanding the charge transfer dynamics in dye-sensitized solar cells (DSCs) is imperative for the development of highly efficient devices. Here we fabricated I^-/I_3^- electrolyte based dye-sensitized solar cells with two novel branched starburst shaped triphenylamine dyes TPAA4 and TPAA5 with broader absorption and higher molar extinction coefficient, which showed power conversion efficiencies of 6.52% and 4.60% respectively. Both the dyes were structurally engineered in such a way to avoid the recombination of electrons from TiO_2. Detailed charge transfer dynamics of the devices were studied by employing extensive perturbation techniques such as electrochemical impedance spectroscopy (EIS), charge extraction (CE) and intensity-modulated photovoltage spectroscopic (IMVS) methods.

Key words: **EIS, Triphenyl amine dyes, Charge recombination**

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DOI: https://dx.doi.org/10.5281/zenodo.1171808

Polymer nanocomposite materials for thermoelectric applications

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Thermoelectricity is the direct conversion of temperature differences to electric voltage and vice versa(1). A good thermoelectric material should have high electrical conductivity to minimize Joule heating, low thermal conductivity to prevent thermal shorting, and a high Seebeck coefficient for maximum conversion of heat to electrical power or electrical power to cooling. Besides being easily processable and scalable compared to the inorganic counterparts, the most conducting polymer has the inherent advantage of having very low thermal conductivity(2). Despite considerable scientific know-how generated in the last decade, the practical implementation of the polymer nanocomposite based devices needed to address important factors like adopting a materials/device fabrication scheme with better batch reproducibility, innovation in device design to maximize power conversion and finding the right interconnects for low-loss transport. Herein, we prepared several polymer-nanocomposite systems and explored their strengths and limitations for practical applications. The polymer components consisted of fused thiophenes, PEDOT and PANI, etc. while single/multi-walled carbon nanotubes and several important inorganic nanostructures (metal QDs, metal oxides, $Bi_2Te_{3,}$ etc.) were used to form the desired composites. For each combination, the percolation threshold for conductivity obtained by varying polymer/nanocomposite weight ratio. Our experiments showed that apart from achieving the right balance of electrical/thermal conductivity and thermo e.m.f., the total device resistance played a crucial role in extracting optimized power output.

polymer, hybrid, nanocomposite, thermoelectrics

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Structural, Magnetic and Thermoelectric Properties of α-MnO_2 synthesized by Hydrothermal Process

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Abstract

α-MnO2 was successfully prepared by hydrothermal technique using potassium permagnet (KMnO4), hydrochloric acid (HCl) and DI water as raw materials. The phase formation of the product was confirmed by using x-ray diffraction (XRD) pattern which shows that the material was exactly manganese dioxide (pyrolusite) with rutile crystal structure, it was further confirmed by Rietveld refinement. Raman spectra also confirm the pure phase formation of the samples. FESEM images were taken to observe the surface morphology of the particles. Vibrating Sample Magnetometer (VSM) was used to evaluate the magnetic properties viz. hysteresis loop (M-H curve, ±50 kOe) and magnetization vs. temperature (M-T curve, 10 - 300 K) in zero field cooling (ZFC) and field cooling (FC) mode with different field values. Hysteresis curve of the sample shows ferromagnetic like ordering at 10 K and also at the same temperature, the coercivity in the sample was observed to be 2.9 kOe and remnant magnetization was observed as 0.34 emu/g. Thermoelectric measurements of these samples show promising material to be used as energy harvesting application.

Keywords: Hydrothermal technique, magnetic properties, ferromagnetic ordering, XRD

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DOI: https://dx.doi.org/10.5281/zenodo.1171820

Structural, Magnetic and TransportProperties of $La_{0.7}Sr_{0.3}MnO_3$-Graphene Nanocomposite

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Abstract

$La_{0.7}Sr_{0.3}MnO_3$(LSMO) polycrystalline sample was prepared using standard solid-state route, pure phase formation was confirmed using x-ray diffraction (XRD) and further supported by Rietveld Refinement. Magnetic properties of LSMO and graphene powder mixed LSMO show enhancement in magnetization as well as Curie Temperature which shows that addition of graphene can also enhance ferromagnetic ordering in the same way as Sr substituted LaMnO3 enhances the magnetic properties owing to presence of double exchange mechanism. Resistivity measurements of LSMO and graphene mixed sample shows high magnetoresistance below Curie temperature.

Keywords: Solid-state route, magnetic properties, X-ray diffraction, magnetoresistance

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DOI: https://dx.doi.org/10.5281/zenodo.1171824

Plasmonic induced effect of Au-graphene-TiO_2 photocatalyst for visible region solar water splitting

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Abstract

Plasmonic Au loaded reduced graphene oxide (rGOs)-TiO_2 photocatalysts were synthesized by using hydrothermal decomposition processes. The graphene oxides (GOs: 0.25-1.0 wt%), Au (1.0-4.0 wt%) and rest TiO_2 were chosen to prepare the Au loaded rGO-TiO_2 photocatalysts. The formation of GOs is confirmed by the observation of D- and G-band peaks at around 1352 and 1596 cm^{-1} in Raman spectrum. The Au nanoparticles loaded on rGO-TiO_2 surface are around 5 nm as observed in TEM. The photocatalytic activity critically depends on the catalyst architecture. The pure TiO_2 evolved small amount of H_2, i.e., 0.58 mmol, whereas the mixing of small amount of GOs (0.5 wt%) in TiO_2 enhanced the value of H_2 evolution up to 1.02 mmol. The maximum value of 1.34 mmol H_2 was obtained in 1.0 wt% rGOs-TiO_2 photo-catalyst in comparison to 0.58 mmol for pure TiO_2. The Au loading further effectively enhanced the H_2 production and 2.0 wt% Au loading on 1.0 wt% rGOs-TiO_2 surface evolved maximum 12.18 mmol of H_2. The enhanced value of H_2 supports that rGOs and Au successfully restrains the recombination rate of reductive electrons and oxidative holes of highly crystalline TiO_2 for efficient H_2 production.

Keywords: Plasmonic, TiO_2, Water Splitting, Gold

DOI: https://dx.doi.org/10.5281/zenodo.1171827

Nanocrystalline silicon oxide immunosensor for toxicity detection in drinking water

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Abstract:

Drinking water is an essential element for human being. Recently, quality testing of drinking water has become a major issue to the people. It has been observed that, due to the presence of toxic components in drinking water severe health problems have been created. Presently, several researches have been focused on water toxicity monitoring. It has been also observed that, the previously reported processes on water toxicity monitoring cannot detect toxic elements below the pg/l range. In this regard, a monitoring system has been developed with nanoporous silicon impedance biosensor followed by a data analysis with a neuro-fuzzy algorithm to detect toxic substances in water samples. The system has a sinusoidal signal generator with frequency from 125Hz to 52 KHz, sensor drive circuit, RMS to DC conversion unit, controller unit and display unit. This system is capable of detecting aflatoxin B2 and ochratoxin-A properly down to concentration level of 0.1fg/ml.

Keywards: Immunosensor, neuro-fuzzy algorithm, water toxicity monitoring.

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DOI: https://dx.doi.org/10.5281/zenodo.1171835

Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials

Hybrid of $MoSe_2$-$Ni(OH)_2$ nanosheets as efficient electrode material for high energy asymmetric supercapacitors

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Abstract

$Ni(OH)_2$ is a promising materials for supercapacitors, but it suffers from capacitance decrease with repeated cycles at high current density. To enhance the specific capacitance and stability performance at high current densities, a newer $MoSe_2$-$Ni(OH)_2$ nanohybrid has been prepared by a simple one step hydrothermal synthesis. The maximized synergistic effect among $Ni(OH)_2$ nanosheets and $MoSe_2$ resulting in its excellent electrochemical properties. The $MoSe_2$-$Ni(OH)_2$ hybrid electrode exhibits a higher specific capacitance of 1175 F g^{-1} at 1 A g^{-1} than $Ni(OH)_2$ nanosheets. In addition, the $MoSe_2$-$Ni(OH)_2$ hybrid based asymmetric supercapacitor provides a high energy density of 43 Wh kg^{-1}, power density of 8181 W kg^{-1} with the capacitance retention of 91.6% even after 5000 cycles at high current density of 5 A g^{-1}. When charged for only 1 min, two asymmetric supercapacitors assembled in series give power to light-emitting-diodes for more than 5 min, indicating the great potential of prepared $MoSe_2$-$Ni(OH)_2$ nanohybrid for excellent energy storage.

Keywords: Molybdenum diselenide, $Ni(OH)_2$ nanosheets, Asymmetric supercapacitor, Cyclic stability

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DOI: https://dx.doi.org/10.5281/zenodo.1171839

Supramolecular Polymers: From Molecules to Materials

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Supramolecular polymer is an important class of soft material because of its exceptional properties like reversibility and stimuli-responsiveness.[1] The unique properties of supramolecular polymers make this fascinating class of material to replace conventional covalent polymers and compare with biopolymers. I will present very recent achievement of light-induced dynamic control over foldability of supramolecular polymer inspired by protein foldability-unfolding. It has been achieved from naphthalene-azobenzene dyad that has an inherent tendency to form folded supramolecular polymer which is unfolded upon UV irradiation.[2] Ferrocene has been used an organometallic scaffold for the tuning of peptide conformation and higher order supramolecular assembly in which the redox state of ferrocene can regulate their material properties.[3] Next, guanosine (G) is conjugated to stimuli-responsive moieties to form G-quartets which afford supramolecular polymers. These supramolecular polymers ultimately lead to the construction of responsive and self-healing hydrogels. Biology mimicking non-equilibrated supramolecular polymer is being constructed.

Keywords: Supramolecular polymer, Soft materials, Responsive materials

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DOI: https://dx.doi.org/10.5281/zenodo.1171844

Raman scattering investigation of stoichiometric and off-stoichiometric Bi_2Te_3 thin films prepared by e-beam evaporation technique

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Abstract

The composition–influenced structural aspects in Bi_2Te_3 thin films significantly influence the thermoelectric properties. E-beam evaporated Bi_2Te_3 thin films and their thermoelectric properties are scarcely explored. Here, we present the Raman spectral investigations on the stoichiometric and off-stoichiometric (Bi-rich and Te-rich) e-beam evaporated nanocrystalline Bi_2Te_3 thin films. Room temperature deposited thin films (BT-AD) are vacuum annealed (BT-VA) at a pressure of 3×10^{-6} mbar and at temperature ranging from 100 °C to 300 °C. The local structural details of the BT-AD and BT-VA films were investigated by Raman spectroscopy using 488 nm laser. The Raman spectra show the infrared (IR) active optical phonon mode (A_1u) is greatly activated. This mode is Raman forbidden in bulk crystals due to its inversion symmetry. Blue shift for A_{1g}^2 and A_{1u} modes for annealing temperatures up to 150 °C, further indicates that the atoms (Bi and (Te) vibrate perpendicular to the layered surface. This could happen mainly due to thinner layers of films. These observations from Raman spectra are correlated to compositional, morphological and crystallite size analysis of BT-AD and BT-VA films using a detailed XRD, FESEM and HRTEM measurements, together with the prediction from the group theory. We attribute the appearance of infrared active (A_1u) Raman spectrum to crystal symmetry breaking of Bi_2Te_3 crystallites in the films. E-beam evaporated thin films and subsequent annealing process provide substantial variable parameters to tailor the structure and composition that will find potential application in thermoelectric devices.

Keywords

Bi_2Te_3 thin films, e-beam, thermoelectric materials.

DOI: https://dx.doi.org/10.5281/zenodo.1171848

Synthesis of orthorhombic MoO_3 nanosheets for visible-light-driven photocatalytic application

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Abstract

Recently, significant attention has been paid to degradation of organic dyes/effluents since the huge utilization of organic dyes/chemicals in the industries which affect the water ecosystem and cause environmental pollution. Thus, thesynthesis ofearth abundant and non-precious metal oxide/sulfidephotocatalysts are highly warranted for large scale photocatalytic applications. Until now, the different semiconductor materials such as TiO_2, ZnO, Fe_2O_3, ZnS, MoO_3 and WO_3have been synthesized and reported as the effective photo catalysts for the degradation of organic dyes (1, 2). Among them, MoO_3has attracted much more attention in various fields due to its layered structure and easily variable oxidation states (3, 4).In this work, sheet like α-MoO_3 nanostructures were synthesized by simple hydrothermal method for photocatalytic applications. XRD results reveal that the synthesized MoO_3 nanostructure is a pure orthorhombic phase(α-MoO_3) with highly crystalline in nature. The characteristic vibration of Mo and O atoms in MoO_3 nanostructure were evidently confirmed by FTIR analysis. The optical band gap energy 3.07eV was calculated from UV-Vis DRS spectroscopy. FE-SEM images indicated that the synthesized α-MoO_3 have sheet like morphology. Furthermore, the synthesized α-MoO_3were used as photocatalyst for the degradation of methylene blue and rhodamine B organic dyes.

Keywords: Hydrothermal method, MoO_3nanostructures, Photocatalyst, Organic dyes

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DOI: https://dx.doi.org/10.5281/zenodo.1171852

Engineering Organic chromophores for Luminescent Solar Concentrators

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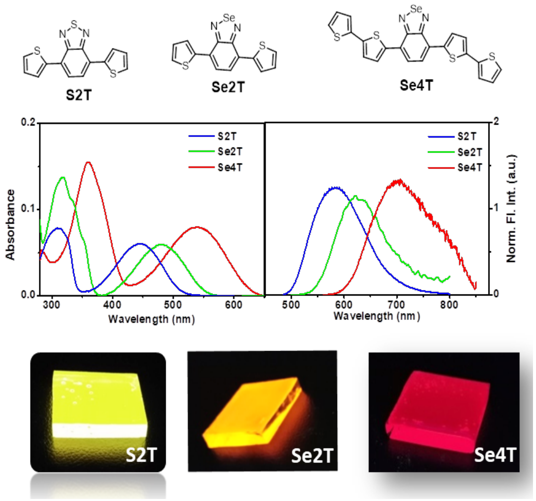
Social and economic development of modern societies strongly depends on the access to a cheap, abundant and relentless supply of energy.Compared to fossil fuels, solar energy satisfies the key requirements for an environmentally-friendly and renewable energy technology, able of reducing the dumping of CO_2 in the atmosphere.It has been estimated that ~ 40 % of the total energy consumption occurs in buildings, 70 % of which in the form of electricity. One method to tackle this issue is by making buildings. In principle buildings can be made self-sufficient in terms of energy needs by integrating solar cells into building infrastructures such as walls and windows (building integrated photovoltaics (BIPVs)).[1]In this context, luminescent solar concentrators (LSC) have emerged as promising candidates for building integrated photovoltaics.[2]



Here we report synthesis and characterization organic chromophores for differently coloured luminscent solar concentrators.The fundamental studies on how their opto-electronic properties affects the performance of LSCs are presented here.

Solar cells, Luminescent solar concentrator, building integrated photovoltaics, organic chromophores

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DOI: https://dx.doi.org/10.5281/zenodo.1171860

Donor-π-AcceptorConjugated Organic Dyes for Efficient Dye-Sensitized Solar Cells.

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Harvesting solar energy is one of the hot areas of current research as they offer greener and sustainable way of meeting the energy needs of the modern society. In this context, photovoltaic cells, devices which convert solar energy directly into electrical energy, are of prime importance. Among the various dye sensitized solar cells (DSSCs) have emerged as one of the leading third generation photovoltaic technologies.[1]The main advantageous of DSSCs are simplicity of design, architecture, and cost effectiveness, and can be easily fabricated with minimum investment. It consists of a photosensitizer (dye) adsorbed onto semiconductor (TiO_2 or ZnO)which act as a photoanode, an electrolyte and a counter electrode.[2]The dye absorbs solar light and transfers an electron to the conduction band of a metal oxide semiconductor.The dye gets regenerated by accepting an electron from the electrolyte which is then revived by the catalytic redox reaction at the counter electrode. The efficiency of DSSCs is mainly determined by the character of the dye employed. Ease of synthesis, ability to tune its opto-electronic properties by structural control, high stability and less toxicity makes completely organic based dyes as promising candidates for this technology. Herein we demonstrate design and synthesis of thiophene based donor-π-acceptor conjugated organic dyes for DSSC applications. The solar cells fabricated out of these simple dyes yielded efficiencies above 8 %.

Solar energy conversion, dye-sensitized solar cells,donor-π-acceptor conjugated organic dyes, renewable energy

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DOI: https://dx.doi.org/10.5281/zenodo.1171866

Effect of cobalt doping on the structural, optical, thermal and mechanical properties of Ammonium Dihydrogen Phosphate single crystals

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Abstract:

Non linear optical single crystals of pure and Cobalt doped ADP were grown by slow evaporation solution growth technique at ambient temperature. The objective of the study is to find out the influence of cobalt on the growth morphology, optical and thermal characteristics of the ADP single crystals. The unit cell dimensions and crystalline nature of the grown crystals were verified by X-ray diffraction technique. The hardness of the crystals was determined by Vicker's Micro hardness test. The optical nature of the grown crystals was analyzed using the UV-Vis spectra. Thermo gravimetric analysis shows the thermal stability of the grown crystals. The addition of Cobalt impurity improves the quality, yield and growth rate of the ADP crystals. The optical quality, thermal and mechanical stability showed the suitability of the cobalt doped ADP crystals for optical applications.

Keywords: ADP, Doping, Cobalt, XRD, Micro hardness

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DOI: https://dx.doi.org/10.5281/zenodo.1171870

Molecular docking and quantum chemical calculation of 4-[(2, 4- dichlropheneyl) amino] 2-methylidene 4-oxo butanoic acid by density functional theory

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Abstract

4-[(2,4- dichlropheneyl) amino] 2-methylidene 4-oxo butanoic acid (DPAB) is regarded as an attractive anti viral agent. To rationalize the detailed interaction between DPAB and its inhibitors at the atomic level, an integrated computational approach by combining molecular mechanics and quantum mechanics methods was employed in this report. The spectroscopic properties of 4-[(2,4-dichlropheneyl) amino] 2-methylidene 4-oxo butanoic acid compound were investigated by FT-IR, FT-Raman spectroscopic techniques. FT-IR (4000-400cm^{-1}) and FT-Raman spectra (3500-10cm^{-1}) in the solid phase were recorded. The structural and spectroscopic data of the molecule have been obtained from DFT (B3LYP) with 6-311++G(d,p) and 6-311+G(d,p) basis set calculations. The geometry of the molecule was fully optimized, vibrational spectra were calculated and fundamental vibrations were assigned on the basis of potential energy distribution (PED) of the vibrational modes. Besides, frontier molecular orbitals (FMO), the molecular electrostatic potential (MEP), nonlinear optical properties (NLO) and Fukui functions were performed.

DOI: https://dx.doi.org/10.5281/zenodo.1171872

Microbial study, molecular docking, Fukui functions and RDG analysis of 3, 4-chlorophenyl acetic acid

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Abstract

The structure and several spectroscopic features along with reactivity parameters of 4-chlorophenylacetic acid (CPA) have been studied using experimental techniques and tools derived from quantum chemical calculations. Structure optimization is followed by force field calculations based on density functional theory (DFT) at the B3LYP level of theory. Local reactivity descriptors such as Fukui functions and local softness's have also been calculated to find out the reactive sites within the molecule. Estimation of biological effects has been made on the basis of prediction of activity spectra for substances (PASS) prediction, docking results and the microbial study also reported. Weak interactions such as hydrogen bonding and Van der Walls interaction were analyzed via reduced density gradient (RDG) analysis in CPA.

DOI: https://dx.doi.org/10.5281/zenodo.1171878

Molecular structure, vibrational spectra (FT-IR and FT-Raman), NBO, Molecular orbital analysis and evaluation of microscopic NLO behaviour of (2E)-1-(4-bromophenyl)-3-(4-chlorophenyl) prop-2-en-1-one

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Abstract

(2E)-1-(4-bromophenyl)-3-(4-chlorophenyl) prop-2-en-1-one (BP4CP) has been optimized by DFT (B3LYP) and LC-DFT (CAM-B3LYP) method at 6-31+G (d). A detailed vibrational spectral analysis was carried out and the assignments of the observed bands have been proposed on the basis of Potential energy distribution (PED). Molecular electrostatic potential (MEP) surface was plotted over the geometry to elucidate the reactivity of the molecule. NBO analysis has been performed in order to demonstrate charge transfer or conjugative interaction and delocalization of electron density within the molecule. HOMO–LUMO analysis has been done in order to determine the way the molecule interacts with other species. On the basis of vibrational analysis, other molecular properties such as ionization energy, electron affinity, chemical potential, global hardness and electrophilicity were also calculated. The electronic properties were determined by time-dependent LC-DFT approach. The microscopic nonlinear optical (NLO) behaviour of the BP4CP has been computed using LC-DFT method. From LC-DFT calculation results, the title molecule exhibits high microscopic NLO behaviour.

DOI: https://dx.doi.org/10.5281/zenodo.1171880

Vibrational Spectroscopic investigation, Magnetic susceptibility, MEP, NBO, NLO, Fukui function and quantum chemical parameters analyses of 1(3, 4-Dichlorophenyl)ethanone

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Abstract

The molecular structure, vibrational spectra, NLO, NBO, MEP and HOMO, LUMO analysis of 1(3, 4-Dichlorophenyl)ethanone were reported. The vibrational wavenumbers were computed using DFT quantum chemical calculation. The data obtained from wavenumber calculations are used to assign vibrational bands obtained experimentally. HOMO and LUMO energies show that the charge transfers occur within the molecule. The Stability of the molecule arising from hyper-conjugative interaction and charge delocalization has been analyzed using NBO analysis. Gauge-including atomic orbital ^{1}H and ^{13}C NMR spectral assessment have been made choosing structure-property relationship by chemical shifts along with the magnetic shielding effects regarding the title compound. The first hyperpolarizability of the title compound is greater than that of the standard nonlinear optical (NLO) material urea and its derivatives are good objects for further research in nonlinear optical analysis. Magnetic susceptibility and thermodynamic properties have been determined for various ranges of temperature. Mullikan's net charges and the atomic natural charges have been calculated. Molecule sites prone to electrophilic and nucleophilic attacks have been detected by the calculation of average local ionization energies, while calculations of Fukui functions have provided additional information about the local reactivity properties.

DOI: https://dx.doi.org/10.5281/zenodo.1171885

Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials

Computational analysis of 2E-1-(Anthracene-9- yl)-3-(4chlorophynyl) by density functional theory

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Abstract

Anthracene is a solid polycyclic aromatic hydrocarbon consisting of three fused benzene rings derived from coal-tar or other residues of thermal pyrolysis. Anthracene is used in the artificial production of the red dye alizarin. It is also used in wood preservatives, insecticides, and coating materials. Anthracene is colorless but exhibits blue (400-500nm peak) fluorescence under ultraviolet light. The structure and several spectroscopic features along with reactivity parameters of anthracene-9-yl-3-(4chlorophynyl) have been studied using experimental techniques and tools derived from quantum chemical calculations. Structure optimization is followed by force field calculations based on density functional theory (DFT) at the B3LYP level of theory. Local reactivity descriptors such as Fukui functions and local softness have also been calculated to find out the reactive sites within the molecule. The geometry of the molecule was fully optimized, vibrational spectra were calculated and fundamental vibrations were assigned on the basis of potential energy distribution (PED) of the vibrational modes.

DOI: https://dx.doi.org/10.5281/zenodo.1171887

DOI: https://dx.doi.org/10.5281/zenodo.1171887

Magneticandmagnetocaloricpropertiesof$YCr_{0.85}Mn_{0.15}O_3$orthochromites

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Abstract

Orthochromites have attracted significant attention of the researchers due to their interesting properties like temperature induced magnetization reversal (TIMR), exchange bias (EB), spin reorientation (SR) and magnetocaloric effect (MCE) along with their potential applications in spintronics, thermally assisted random access memory and magnetic refrigeration devices [1-2].We have investigated structural, magnetic and magnetocaloric properties of manganese (Mn) doped$YCr_{0.85}Mn_{0.15}O_3$ (YCMO) polycrystalline compoundwhich possesses orthorhombic unit cell with *Pnma* space group.EDXanalysisconfirmed the basic constituents of YCMO compound. The compound showed the Neel temperature (T_N) ~ 132 K, lower than that for pristine YCO sample. It also exhibited negative magnetization around 52 K in field cooled (FC) mode. The magnetic entropy change, ($-\Delta S$) ~ 0.365J kg^{-1} K^{-1}along with relative cooling power (RCP) ~ 13.52J kg^{-1}, wasobtained near 36 Kunder an applied field of 9 T.

Keywords: Orthochromites, magnetization reversal,magnetocaloric effect

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DOI: https://dx.doi.org/10.5281/zenodo.1171889

Bio-synthesized Hydroxyapatite Nanoparticles for Sensor and Antimicrobial applications

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Abstract

Hydroxyapatite ($Ca_{10}(PO_4)_6(OH)_2$, HA) is the main mineral constituent of natural bone and teeth. It attracts considerable interest in many areas because of its acid-base properties, ion-exchange ability, biocompatibility and adsorption capacity. A great variety of cationic and anionic substitutions in HA is possible due to its "open structure'' [1]. The characteristics of HA NPs depend on the method of synthesis which influences particle size, shapes and phase purity. A number of novel processing routes such as dry, wet, hydrothermal, sonochemical, and microwave assisted process have been developed for preparing HA powders [2]. Chemical method may successfully produce pure, well-defined nanoparticles, these are quite expensive and potentially dangerous to the environment. On the other hand, biosynthetic methods employing either biological microorganisms or plant extracts are simple and eco-friendly. Here we report to synthesis HA Nps by using different plant extract such as Eucalyptus, Ocimum basicilium, Plectranthus amboinicus, and Jusiticia adathoda by microwave method. Biosynthesized HA Nps were successfully applied to fabrication of sensor and antimicrobial application. The Electrochemical behavior of 2-Nitrophenol was investigated by cyclic voltammetry (CV), differential pulse voltammetry (DPV) techniques by using pristine HA and plant extracts assisted HA Nps modified GCE. Among them, Plectranthus Amboincus assisted HA Nps modified GCE exhibits excellent electro catalytic activity towards 2-Nitrophenol. Moreover, it has been good sensitive for determination of 2-Nitrophenol over a wide linear range from 0.2µM to 60µM with the lowest limit of detection 90nM. The nanoparticles samples were evaluated against *S. aureus*, *S. mutants, P. aeruginosa* and *E. coli* species. The inhibition of zone for bacterial species most significant effect of tested range from 13 to 21mm of *S. mutants,* and *E. coli* 11 to 17mm. The highest inhibition of zone was observed in gram-positive bacteria, due to the van der Waals interaction (electrostatic interaction) between accessible negatively charged bacterial cell membrane and positively charged nanoparticles.

Keywords: *Hydroxyapatite nanoparticles; Plectranthus amboinicus; Sensors; Antimicrobial activity;*

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DOI: https://dx.doi.org/10.5281/zenodo.1171893

DC Electrical Conductivity and Band Gap TailoringforSn Doped TiO_2Nanoparticles

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Abstract: Materials in nanoscale can exhibit sensational results with small variation in its state with many applications in nanoscale devices. Doping is one of the techniques to vary the band gap as well as size of the nanoparticles, attempt has been made to control the band gap and size of the nanoparticle by doping Sn to TiO_2 nanoparticles synthesized by peptization method. From XRD and SEM images it confirms the crystallinity and surface morphology.The structural parameters and the size of the particle can be controlled by appropriate amount of doping in to host lattice. Theparticle size varies between 40.5nm to 92nm for the doping concentration 10% to pristinerespectively, EDAX peaks showsthere is no extra phase**,** UV-spectra and Tauc plot confirms the tailored band gap of the material varies from 2.99eV to 3.09eV.These samples were subjected to DC Electrical conductivity studies from RT to400°C,from Arrhenius plot clearly we encountered activation energy starts from 0.29 eV to 1.69eV for pristine to 10% doped sample respectively, decrease in the conductivity for the decrease in particle sizedue to hopping of charge carriers and it dominant with phonon scattering phenomenon. In partly reduced TiO_2, oxygen vacancies are formed in the oxygen ion lattice which in turn ionizes to form free electrons, due to this there is an increases in the conductivity with temperature and show the semiconductor nature of the prepared sample.

Keywords: Peptization; Crystallinity; Tauc plot; Arrhenius plot.

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DOI: https://dx.doi.org/10.5281/zenodo.1171898

Synthesis and Acetone Sensing Properties of Porous CeO_2 Nano particles.

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Abstract

CeO_2 Nano particles with a porous morphology were successfully prepared through solution combustion method at 400°Cwith subsequent calcination. X-ray diffraction confirms the formation of crystalline phase along with particle size less than 22nm. The field-emission scanning electron microscopy reveals the surface morphology of the material, EDAX and UV were used to analyse the elemental composition and optical band gap prepared samplesrespectively. Gas sensing analysis revealed that the CeO_2sensor showed excellent response and selectivity to acetone with quick response and recovery times, which might substantially benefit from their distinctive porous structure and large surface area.

Keywords

CeO_2nano particles;Acetone; Gas sensors

DOI: https://dx.doi.org/10.5281/zenodo.1171900

Plasmonic Metal Nanostructure Modified $BiFeO_3$HeterostructuredPhotocatalystfor Visible Light Driven Photocatalytic H_2 Generation

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Abstract

Visible light active photocatalysts can offer a green approach to solve renewable energy production by solar light harvesting. In this regard, perovskite based oxide are considered as novelcatalytic material for photochemical water splitting (1). However, the low charge separation efficiency and fast recombination rate lowers the catalytic efficiency (2). In this work, we overcome the aforementioned problems by decorating the ferroelectric $BiFeO_3$ (BFO) surface with plasmonic Au nanoparticles (NPs) to increase optical absorption in visible region. Herein, single crystalline BFO nanosheets (400 nm) have been successfully prepared by hydrothermal method and Au NPs (~ 17 nm diameter) have been introduced on the BFO hexagonalnanostructure*via* radiolysis process without using any toxic reducing agents. The as-synthesized materials have been used as the photocatalyst for hydrogen generation under visible light and the experimental result reveals that Au/BFO heterostructures are more efficient in water splitting compare to bare BFOnanosheets.

Keywords:Perovskites, Plasmonic metal nanoparticles, Heterostructures, Visible light active photocatalyst, H_2 generation

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DOI: https://dx.doi.org/10.5281/zenodo.1171906

Preparation and characterization of $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ for anode application in solid oxide electrolyser cell

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Abstract

Solid oxide electrolyser cell (SOEC) has the great potential for efficient and economical production of hydrogen fuel via high temperature steam electrolysis. It is one of thecleanest methods to produce hydrogen. An SOECconsists of an ion conducting solid electrolyte sandwiched between two porous electrodes.Steam is introduced at the cathode where it is reduced into H_2, releasing oxide ions which move through the electrolyte to the anode where they combine to form O_2 molecules, releasing electrons. One of the key issues related to the performance of SOEC is the stability of the electrodes under electrolysis conditions (1,2). Therefore, intensive research is being carried out throughout the world to develop stable and highly active electrodes for SOEC application.

Under the present work, $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$(BSCF) has been prepared for its application as an anode material in SOEC.The materialis synthesized through combustion synthesis technique using glycine and /or citric acid as the fuel and corresponding nitrate salts of the metals.Critical process parameters such as fuel to nitrate ratio, metal ion concentration, pH, temperature etc have been optimized. XRD analyses reveal that single phase perovskite of BSCF is obtained at 950°C. Bulk samples have been fabricated through uni-axial compaction of the calcined powder followed by sintering in the range 1250-1400°C. The sintered samples have been characterized through thermal expansion coefficient (TEC) measurements, microstructural analysis and electrical conductivity measurements. Finally, single cell of configuration (BSCF-GDC/YSZ/Ni-YSZ) has been fabricated using tapecasting and screen printing techniques. The performance evaluation of the fabricated single cells (16mm diameter) is currently under progress.

Keywords: Solid oxide electrolyser cell, BSCF, perovskite

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DOI: https://dx.doi.org/10.5281/zenodo.1171909

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DOI: https://dx.doi.org/10.5281/zenodo.1171909

Optical properties of $Dy_xTi_{1-x}O_2$ nanocomposites

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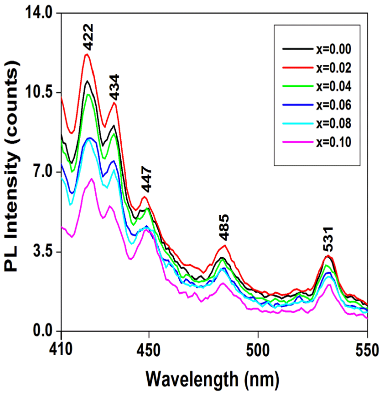
Abstract

$Dy_xTi_{1-x}O_2$ nanocomposites with X=0-0.1 are obtained through sol-gel method. The prepared sample is annealed at 450˚C for 2 h and characterized using DRS and PL spectra. The absorbance spectra of $Dy_xTi_{1-x}O_2$ nanocomposites, compared to pure titania, show red shift in the band-gap transition which can be attributed to the charge-transfer transition between Dy^{3+} ion f electrons and the TiO_2 conduction or valence band. The absorption hump seen at 701 nm reveals the visible-light absorbability of these nanocomposites. This peak is attributed to the 4f electron transitions of Dy^{3+} ions. The tauc plot gives indirect band gap of $Dy_xTi_{1-x}O_2$ nanocomposites and are 3.212(1), 3.187(1), 3.157(2), 3.143(1) and 3.142(1) for x=0.02, 0.04, 0.06, 0.08 and 0.10 respectively. It has been observed that the band gap decreases with the increase in Dy inclusion. From PL spectra several emission bands are observed including violet emissions at 422 & 434 nm, blue emission at 447 nm, blue-green emission 485 nm and green emission 531 nm were observed. These emissions are assigned to the surface state emissions and due to the recombination of trapped electron-hole arising from dangling bonds in the TiO_2 nanoparticles. With the increase of Dy concentration, intensity of the PL emission has decreased as in Figure 4.8. The decrease in the PL intensity ensures the separation of charge carriers. This clearly indicates that these $Dy_xTi_{1-x}O_2$ nanocomposites have a better light-absorbing ability than bare TiO_2 since it absorb the visible light, which makes them a potential visible light photocatalyst.



Keywords: nanocomposites; optical properties; 4f transition

DOI: https://dx.doi.org/10.5281/zenodo.1171911

Effect of Nanostructured Binary Metal Sulfide (CoS) on its Magnetic and electrochemicalbehavior for Supercapacitance Applications

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Abstract

Metal sulfides are ofgreat interest for future electrode materials in supercapacitor applications owing to theirsuperior electrochemical activity and excellent electrical conductivity. With this scope, a binary transition metal sulfide (CoS) is prepared via template assisted one-step hydrothermal synthesis. Hexagonal phase of CoSwith the space group of $P6_3/mmc$ (194) is confirmed by X-Ray diffraction analysis. The morphological features are visualized using HRSEM results that shownanoflower shaped morphology which agglomerated to form ascluster. The magnetic behavior of the prepared sample was measured using vibrating sample magnetometer which revealed clear hysteresis loop (M-H loop) with paramagnetic nature upto 125 K. At low temperature 2 K and 10 K, the paramagnetic nature gets transformed to ferromagnetic behaviorwhich is further evidenced with the M-T curve. The interfacial charge transport kinetics was examined by EIS-Nyquist plot byemploying the prepared CoS as active electrode material.The supercapacitive performances were tested in three electrode system and the estimated specific capacitance for 1A/g is 348 F/g.

Keywords: Binary metal sulfide; CoS; Electrochemical impedance spectroscopy; Supercapacitance.

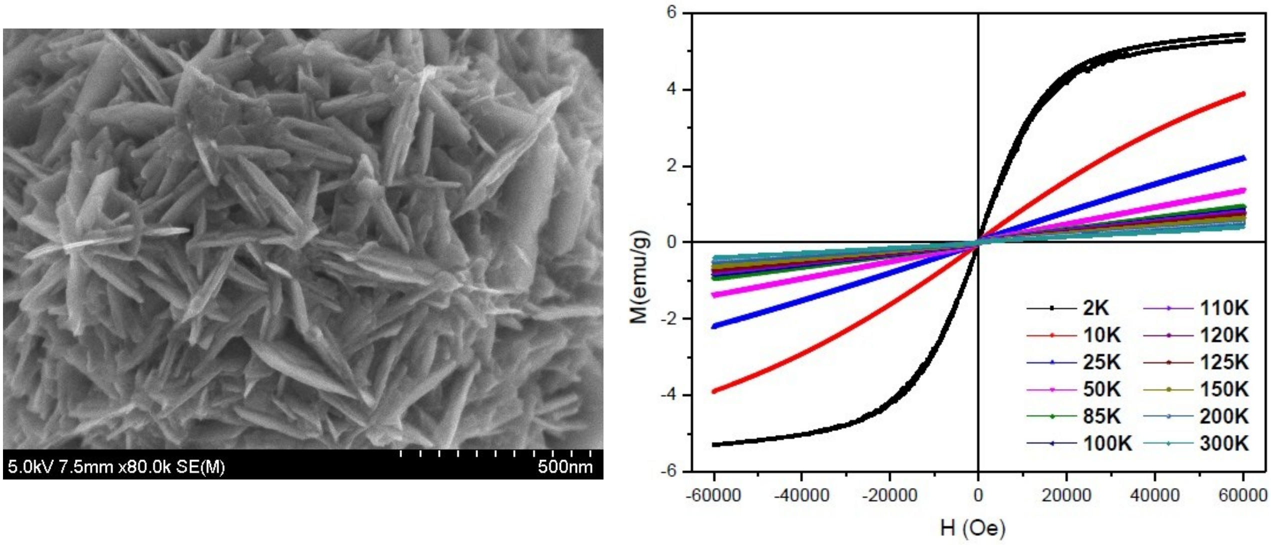

Fig: HRSEM image of CoS and temperature dependent M-H curve

DOI: https://dx.doi.org/10.5281/zenodo.1171913

Beta Gallium Oxide Nanowires and Nano-sheets growth by Chemical Vapour Deposition

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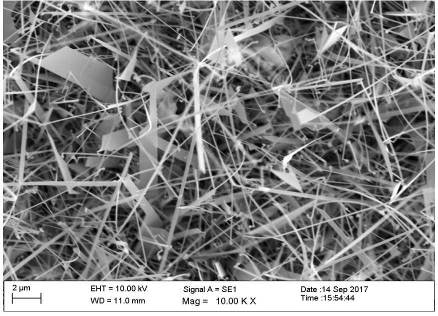
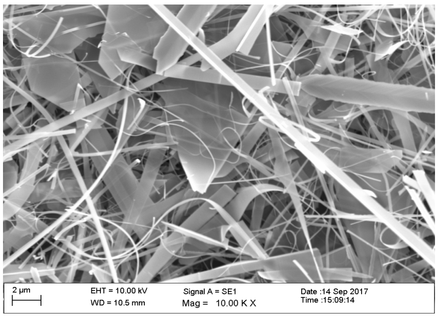
Abstract

One dimensional and Two dimensional semiconductor nanostructures have taken much consideration of researchers due to its potential device applications [1-2]. The wide band gap (E_g : 4.9 ev) and Monoclinic structured beta gallium oxide (β -Ga2O3) is an important material for the applications including TCO, optical emitter for UV, and gas sensors because of its good chemical stability at high temperature [3].

In this work, we have synthesized β-Ga2O3 nanowires and nano-sheets on substrates by the method of chemical vapour deposition at the temperature of 900º C have been reported. Gallium metal serving as the gallium source and argon gas helps to carry the oxygen gas for the nanostructures growth. Initially Au was sputtered on cleaned substrates, which act as the catalyst to assist the growth. X-ray diffraction (XRD) has been used to study the crystal structures of these nanowires and nano-sheets. Scanning Electron Microscope (SEM) images show the formation of nanowires and sheets. Diffuse Reflectance spectroscopy measurements gave the band gap of 4.69 ev for these nanostructures. Energy Dispersive X-Ray Spectroscopy (EDX) has shown the elemental compositions of gallium oxide deposited samples.





Keywords: β-gallium oxide nanostructures, Powder X-Ray Diffraction, Scanning Electron Microscopy, Diffuse Reflectance Spectroscopy.

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DOI: https://dx.doi.org/10.5281/zenodo.1171917

Development of $NiTiO_3$Nanofibers by Sol-Gel Supported Electrospinning

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Nanofibers of transition metal oxides are familiar as intelligent materialsfor one dimensional nanostructure. In this study, we report that the $NiTiO_3$ nanofibers were prepared by sol-gel supported electrospinning method. These nanofibers were calcined at 450^0C to produce the NTO nanofibers. The SEM results revealed that the surface of the nanofibers are uniform and smooth, the fibers diameter got decreased after the calcination. The XRD analysis shows that the nanofibers possess rhombohedral structure. From the AFM images, it was confirmed that the as-prepared Nano Fibers have smooth surface, whereas the calcined Nano Fibers were not obtained because of the difficulty due to the roughness of the sample.

Keywords:Electrospinning, Nanofibres, Transition metal oxides.

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DOI: https://dx.doi.org/10.5281/zenodo.1171921

Synthesis and Characterization of Enhanced Luminescent Properties of CdTe Quantum Dots

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Abstract

Quantum Dots (QDs) are semiconductor nanoparticles which have unique optical and photo physical properties. These properties make them widely to be used for fabrication of photovoltaics, optoelectronic devices such as solar cells, electrodes in Liquid Crystal Display (LCD's), Light Emitting Diodes (LED's) and Laser Diodes. Synthesis of quantum dots with increased quantum yield has proved helpful for optoelectronic applications. In this present work, the CdTe quantum dots are synthesized by aqueous phase medium with the Mercaptosuccinic acid (MSA) used as a capping agent. The reaction parameters were optimized to produce highly luminescent MSA-CdTe quantum dots. The size dependent optical properties of MSA-CdTe quantum dots were revealed by UV-Vis absorption analysis. The result shows that the calculated band gap value of the CdTe quantum dots are decreasing with the increase in refluxing time. Emission properties of MSA-CdTe quantum dots were revealed by photoluminescence analysis. Optical band gap values of MSA-CdTe quantum dots for different refluxing time was calculated from the emission spectra obtained. The FTIR analysis confirms the capping of MSA on to the surface of CdTe quantum dots and peaks obtained stands well in agreement with bonding of MSA to CdTe. The crystalline structure of the prepared MSA-CdTe quantum dots were studied by X-Ray diffraction analysis which confirms the cubic zinc blende structure. Thermal stability of MSA-CdTe QDs was analyzed by TGA. Hydrodynamic diameter of MSA capped CdTe QDs was found in the range of 3-10 nm by using DLS. HRTEM results shows the CdTe QDs are having the range of 2-5 nm. The result will be discussed in detail.

Keywords: **Quantum Dots, Mercapto succinic acid, Optical Properties, Photoluminescence**.

Reference: Arivarasan Ayyasamy et al, J. Superlattices and Microstructures 88 (2015) 634-644.

DOI: https://dx.doi.org/10.5281/zenodo.1171929

Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials

Highly green luminescent of indium doped CdTe colloidal quantum dots

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Abstract

Quantum dots gains enhancing interest in scientific and industrial area for optoelectronics applications (1) due to its unique optical and electrical properties such as bandgap tunability, high absorption coefficient, multiexciton generation, delivery of hot electrons (2) and also low cost and solution processability (3). This research work describes the colloidal synthesized of 3-Mercaptoproponic acid (3-MPA) capped CdTe QD and Indium doped (1%, 3%, 5%) CdTe quantum dots were accomplished. All these procedures were carried out in aqueous medium at air atmosphere. Highly green luminescent of CdTe and Indium doped CdTe colloidal quantum dots of size dependent band gaps were determined from UV-Vis spectra. The photoluminescence properties of the prepared quantum dots were characterized by using photoluminescence spectroscopy. The structural and morphologies were studied by HRTEM and X-Ray diffractometer. The formation of Indium doped quantum dots and the capping effect of the thiol group was investigated by using FTIR studies. Using DLS the particle Size ware analyzed.

Keyword: Quantum dots, Optoelectronics, CdTe, Doping

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DOI: https://dx.doi.org/10.5281/zenodo.1171931

δ-UZr_2 : Structural stability & thermal expansion coefficient at HP-HT

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Abstract

UZr_2 exhibits cubic *bcc* phase at high temperature known as γ-UZr_2 and modified AlB_2 type hexagonal phase at ambient known as δ-UZr_2 (1, 2). HP studies up to 20 GPa on δ-UZr_2 reveals the structure to be stable and bulk modulus is estimated to be 108 GPa. An anomalous increase in the rate of change in *c/a* ratio has been observed beyond 10 GPa. From structural stability computation, this is understood to be due to the strengthening of U-Zr bond, along *a*-axis at lower pressures. The localization of charge density at high pressures indicate decrease in metallization of the material which is in contrast to the usual behavior of the materials at high pressure. *In-situ* HP-HT XRD studies (3) on δ-UZr_2 have been carried out up to 6 GPa and 473 K. The structure is found to be stable and the system exhibits softening as expected. However, *c/a* ratio is found to increase with pressure at high temperatures. Thermal expansion coefficients are estimated and show decreasing trend with pressure.

Keywords - High Pressure, High Temperature, DFT computation, Thermal expansion coefficient

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DOI: https://dx.doi.org/10.5281/zenodo.1171935

Effect of Substrate Temperature on the Properties of CuZnS Thin Films Prepared by Vacuum Spray Pyrolysis

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Abstract

Copper Zinc Sulphide (CZS) thin films have been deposited on a glass substrate at different temperatures using Chemical Spray Pyrolysis technique under a vacuum of 10^{-3} Torr. The influence of substrate temperature on the structural, morphological, optical and electrical characteristics of CZS thin films are investigated and reported. The major advantage of this material is that it uses earth-abundant and low-cost constituent elements like Copper, Zinc, and Sulphur. The band gap of the as-deposited films are obtained in the range of 2.36 to 3.2 eV, which makes it a good absorber as well as window layer. The band gap was found to increase with increasing Zn concentration. Structural analysis shows highly crystalline nature with a mixed phase of CuS-ZnS. SEM image shows the homogeneous distribution of closely packed grains without any gap in between. EDX data clearly shows the peaks corresponding to Cu, Zn, and S. The optical properties of the films were studied using UV-Vis-NIR spectrometer. A peak shift has been observed on increasing the substrate temperature of the films. The electrical properties have been investigated using Hall measurement system and all the samples are found to have P-type conductivity.

Keywords: Copper Zinc Sulphide; Vacuum Spray Pyrolysis; p-type semiconductor

DOI: https://dx.doi.org/10.5281/zenodo.1171941

Effect of Substrate Temperature on RF Sputtered NiO thin films

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Abstract:

Nickel oxide (NiO) thin films are deposited by RF sputtering process and the physical properties are investigated for various substrate temperatures. The structural, optical and electrical properties of NiO thin films under varying substrate temperatures are reported in this work. The variation of the crystallographic orientation and microstructure of the NiO thin films with increase in substrate temperature are studied using XRD. It was observed that NiO thin films deposited at 350 ºC shows relatively good crystalline characteristics with a preferential orientation along (111) plane. SEM and AFM investigations unveil that the microstructure of the thin films improves at higher substrate temperatures. Increase in transmittance is observed for NiO thin films upon increasing the substrate temperature. It is revealed that films prepared at substrate temperature of 350 ºC, the NiO films showed higher electrical conductivity which can be utilized for a range of applications as transparent conducting oxides (TCO's) with stable p-type characteristics.

Keywords: Nickel Oxide; RF sputtering; p-type semiconductor

DOI: https://dx.doi.org/10.5281/zenodo.1171945

Oxygen partial pressure dependent tuning of Cu_2O & CuO thin films by Reactive RF Magnetron Sputtering.

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Abstract:

Nanostructured Cu_2O & CuO thin films are deposited on glass substrates by radio frequency (RF) magnetron sputtering using a Cu metal target in an Ar and O_2 reactive atmosphere at 50W of RF power. The functions of oxygen partial pressure in the deposition of Cu_2O & CuO thin films were studied at fixed substrate temperature of 300^0C. The structural, morphological, optical and electrical properties of the deposited thin films were investigated by using X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), UV–Vis spectrophotometry and Hall effect measurement system. The XRD results shows that Cu_2O crystalline phase is obtained at 5% oxygen partial pressure and the phase changes to CuO on increasing the oxygen partial pressure above 10%. SEM images reveal that the deposited thin films are highly uniform. The optical band gaps of as-deposited Cu_2O and CuO samples are 2.18 eV and 1.83 eV respectively. The electrical conductivity of the films obtained using Hall measurement as $1.42x10^{-1}$ $(\Omega.cm)^{-1}$ for Cu_2O and 1.39 $(\Omega.cm)^{-1}$ for CuO samples.

Keywords: Copper Oxide; Reactive RF sputtering; p-type semiconductor

DOI: https://dx.doi.org/10.5281/zenodo.1171950

Structural, Optical, Thermal and SEM studies of Pure and Ferric doped Potassium Penta Borate (KB5) Single Crystals

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Abstract

The development of lasers has played a key role in the past five decades for the development of mankind in various fields and to reach several technological advancements. The demand for laser beams in the ultraviolet and visible regions is growing enormously. The laser beams in the UV and visible regions find applications in several industries, medical surgeries, data storage, optical communication, and entertainment purposes. Advances in semiconductor photolithography, for example, are creating demand for 158 and 193 nm coherent light sources, while emerging micromachining and material-processing applications also need deep-UV laser radiation. In addition, research scientists would like a widely tunable coherent light source down to 200 nm for laser spectroscopy and photochemical synthesis [1]. Potassium pentaborate (KB5) is a desirable inorganic nonlinear optical material which exhibits a low angular sensitivity and hence, proved useful for second harmonic generation (SHG) [2]. Highdamage threshold and wide transparency make it a better alternative for KDP crystals in frequency doubling and laser fusion experiments [3]. A single crystals of pure and Fe doped KB5 were harvested by slow-solvent evaporation techniques. The crystal structure is confirmed by Powder XRD. The optical absorbance studied by UV-Vis. The thermal behavior of pure and Fe doped KB5 discussed by TG-DTA spectrum. Surface studies are discussed by SEM studies.

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DOI: https://dx.doi.org/10.5281/zenodo.1171955

Simultaneous oxidation and reduction of GO and $KMnO_4$ for synthesis of RGO-Mn_3O_4 hybrid electrode material for supercapacitor application

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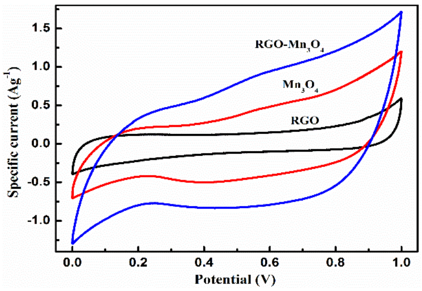
Abstract

RGO-$Mn_3O_4$was synthesized through reflux method. Structural, morphological and electrochemical studies were carried out using XRD, FT-IR, SEM, micro-Raman, cyclic voltammetry, galvanostatic charge/discharge and electrochemical impedance spectroscopy.RGO-Mn_3O_4had a maximum specific capacitance of 158 Fg^{-1} in 1 M Na_2SO_4 electrolyte at the scan rate of $5mVs^{-1}$. The preparedelectrode has>100% specific capacitance retention and Coulombic efficiency evenafter 3000 cyclesat 10 Ag^{-1}. The electrochemical performance confirmedthat the RGO-Mn_3O_4composite,has the positive synergisticeffects between RGO and Mn_3O_4. The as-prepared RGO-Mn_3O_4composite can be used as a hybrid electrodein electrochemical energy storage applications.



Keyword: cyclic voltammetry (CV), specific capacitance, reduced graphene oxide (RGO), electrochemical impedance spectroscopy (EIS).

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DOI: https://dx.doi.org/10.5281/zenodo.1171961

Cresol Novolak Photoresists: Effect of Compositions, Fractionation and Oligomer concentration on Patterning Potential for Thick Film

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Novolak resists have been widely used in making electronic circuits for ICs and VLSIs at micron and sub-micron levels. As advances in electronic systems with higher speeds, greater functionality, and higher densities have generated requirements for higher sensitivity, higher resolution, and wider process margin for novolak resists. In the present work, with the goal of improving the performance of novolak resists, *m, p*-cresol formaldehyde novolak resins have been synthesized by varying the relative amount of cresol monomers. FTIR, ^{1}HNMR and ^{13}CNMR were used to analyze the synthesized resins. GPC was used to determine the molecular weight. Highly fractionated novolak resins (Mw 17000) and low molecular weight novolak resin (Mw 700) at various composition have been investigated for resist formulation to improve resolution and sensitivity. Addition of low molecular weight novolak to highly fractionated novolak enhanced the dissolution rate, fine thin film, image contrast of the resist. Lithographic pattern of resolution 450 nm was observed for cresol novalak of m/p ratio 32/68 and for high fractionated novolak/low mol wt. novolak of 65/35.

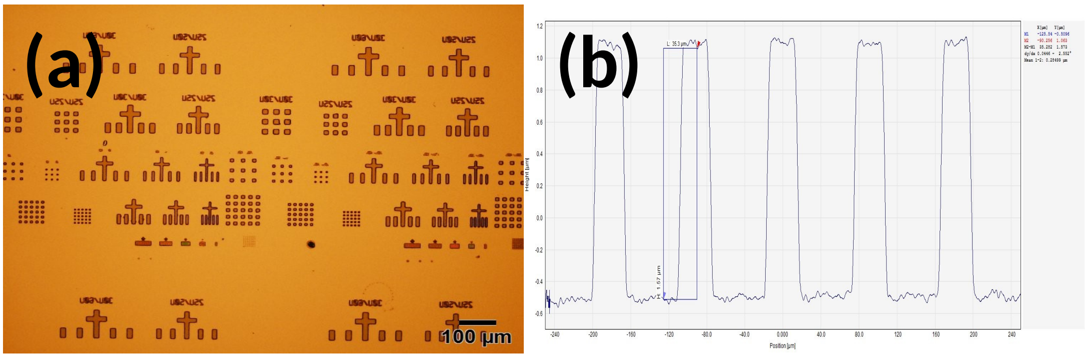

Fig: (a) Lithography pattern and (b) Thickness profile of m/p cresol formaldehyde novolak resist

Keywords: Optical lithography, Cresol novolak, fractionated resin, PAC incorporation

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DOI: https://dx.doi.org/10.5281/zenodo.1171971

Optimizationof molecular weight distributionin terpolymerDUV Photoresists.

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Polymeric photoresists have drawn considerable attention during the last many decades. Photoresist technology as a step in the microlithography process can help to create faster and smaller devices. In the area of polymer materials, ter-polymerization is one of the most important means to improve the properties of existing polymer and to develop new polymers. The end-use properties of polymers are largely dependent on their molecular weight distribution. Molecular weight distribution is an essential parameter to obtain polymers with desired properties. Recently, studies on molecular weight distribution have been the focus of increasing attention, A change in the molecular weight leads to changing in fundamental properties of photoresist. Herein, we demonstrate the simple procedure for optimization of molecular weight distribution of a terpolymerDUV photoresist by changing the concentration of AIBN in a polymeric solution without using additional inhibitors. Traditional photoresist using 248 nm UV wave length resolve features between 0.25-0.18µm.

A terpolymer was synthesized by polymerization of 4-hydroxystyrene, styrene, and t-butyl acrylate with different concentrations of AIBN.

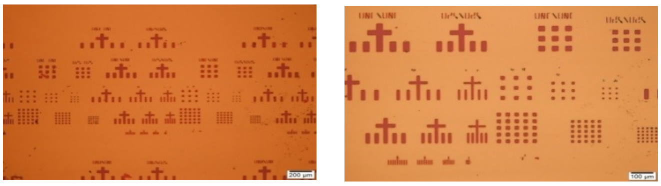

Fig: Lithography pattern of polymer

Keywords : DUV Resists, molecular weight , optimization.

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DOI: https://dx.doi.org/10.5281/zenodo.1171973

Band topology evolution and signatures of Lifshitz transition in $WTe_{2:08}$ nanosheets

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Weyl semimetals have recently attracted a lot of attention due to its unique electronic band structure. They are analogs to Graphene in 3D with vanishing density of states at the band touching point with linearly dispersing energy-momentum relation. The Weyl semimetals are protected by the topological property of the Weyl nodes which act like the source of Chern fluxes in the momentum space. The projection of Weyl nodes on to the surface Brillouin Zone gives rise to Fermi arcs. The unusual band topology of Weyl semimetals is predicted to exhibit different quantum phenomena. Weyl semimetals are further classified into type-I and Type-II based on their band structures. WTe_2 is a newly discovered type-II Weyl semimetal known for extremely large magnetoresistance. Shortly, after the discovery, several experiments came up with the results where a bulk WTe_2 crystal is electronically a lot different from a monolayer.

Here, I will discuss the evolution of band topology of Weyl semimetal $WTe_{2.08}$ nanosheets through transport analysis. We observed a resistivity anomaly in ρ_{xx} Vs. T curve which has not been seen in WTe_2 systems. The resistance anomaly temperature increases as the thickness increases implying the suppression of one type of carrier in the semimetallic band. The evolution of Hall data from non-linear to linear with the decrease of thickness suggests the shifting of the energy bands i.e., from a two-carrier system to a single carrier system. The single carriers being hole carriers suggests the downward shift of the Fermi level. Along with that, we also observed the temperature dependance of individual samples where for thicker samples the Fermi level moves from two bands to a single band system as the temperature increases. At the resistivity anomaly temperature (T^*), where the system enters from a two-carrier system to a one-carrier system signals the presence of a Lifshitz transition. Combining with Hall data and zero-field resistivity Vs. T behavior, we identify the contributions from a semiconducting and a semimetallic band. Finally, our experiments provide an insight into the band structure sensitivity of the WTe_2 system towards thickness and temperature along with that a slight variation of composition which might be the possible reason for its unusual and divergent behaviour.

DOI: https://dx.doi.org/10.5281/zenodo.1172074

Structural, surface morphological and spectroscopic study on cobalt sulphate

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Abstract

The Cobalt Sulphate ($CoSo_4$) is a transition metal group compound. It is used as a coloring and dehydrating agent in the electroplating and electrochemical industries; as a dehydrated agent for lithographic inks, varnishes, paints, in storage batteries and as a dyeing agent in ceramics, enamels, glazes and porcelain(1,2). In the present study, $CoSo_4$ has been characterized by EDXA, SEM, XRD and UV-VIS. The EDXA study confirms the elemental composition and SEM analysis has shown almost spherical nature of the particles. The XRD study confirms the crystalline nature of the compound. The UV-VIS reflectance study shows almost constant high reflectance from 190nm to 350nm. Then decreases and reaches low value at 511nm then again decreases. The behavior is almost like trough from 350nm to 750nm. This may be used in optoelectronic applications. The UV-VIS study deduces the energy gap as 2.14 eV and urbach energy value as 0.3158 eV.

Keywords: Cobalt Sulphate, EDXA, SEM, XRD and UV-VIS

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DOI: https://dx.doi.org/10.5281/zenodo.1172076

Effect of hydrostatic pressure on Transport properties of Mn-site doped $La_{0.5}Ca_{0.5}Mn_{1-x}Mo_xO_3$ (x = 0.03, 0.05) manganites

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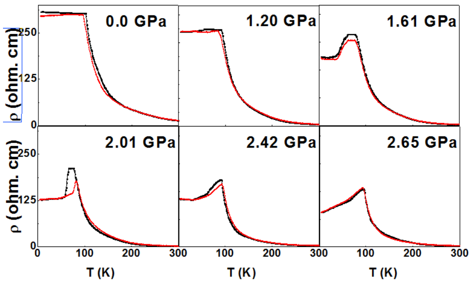
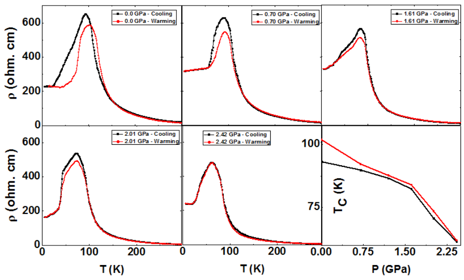
Abstract

The basic character of manganites is mainly due to double exchange (DE) between Mn^{3+} and Mn^{4+}, and this could be modified by doping at A and/or Mn site of the main compounds [1]. We have investigated the transport properties of $La_{0.5}Ca_{0.5}Mn_{1-x}Mo_xO_3$ (0.03 and 0.05) compounds under hydrostatic pressure up to ~ 2.5 GPa. At ambient pressure, x= 0.03 sample exhibits insulator to semiconducting transition around 100 K, whereas x=0.05 sample exhibits insulator to metallic transition around 100 K. It suggests that the enhancement of conductivity through the partial substitution of Mo by Mn, and destroys the charge-ordering (CO) semi conducting phase which induces the metallic transition in $La_{0.5}Ca_{0.5}MnO_3$ at low temperatures. However, the appearance of thermal irreversibility between cooling and warming cycles in both samples suggest the first-order transition, and hence possesses the phase transformation in accordance with latent heat [2]. The pressure on both samples further reduces the resistivity down to low temperature 4K. At the same time, pressure suppresses the hysteresis between cooling and warming cycles of both samples, which leads to change from first-order to second-order transition without change in transition temperatures..



ρ vs T under various P of $La_{0.5}Ca_{0.5}Mn_{1-x}Mo_xO_3$(x= 0.03



ρ vs T under various P of $La_{0.5}Ca_{0.5}Mn_{1-x}Mo_xO_3$(x= 0.05)

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Crystal Growth, Crystal Structure, Phase Transition and Optical Properties of 5FSA

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Abstract:

Organic crystal of 5-fluorosalicylaldehyde with Aniline were grown by solvent evaporation techniques at room temperature. The grown crystals were characterized through single crystal X-ray diffraction study and TG/DSC study. The crystal structure analyzed by single XRD and the crystal system is monoclinic system and the unit cell parameters are Space group=p2_1lc, a=18.965(2), b=4.7214, c=12.2399, β =107.881(7),V(A^3)=1043.0(2), Z=4. TG/DSC studies confirm that phase transition. DSC was taken to study the structural phase transitions occurring in the crystals. The TG curve of the sample shows a prolonged decomposition from 73.2^{0}C and 210 °C, from which the decomposition pattern has been formulated. The endothermic peaks in the DTG curve indicate melting and decomposition of the compound at 296.2^{0}C and 388 °C respectively. An exothermic peak in low temperature DSC indicates a phase transition in the compound at 73.2 °C. The crystal shows three transitions above room temperature.

Keywords

Crystal structure, phase transition, TG/DSC, Thermal analysis and 5-FSA

DOI: https://dx.doi.org/10.5281/zenodo.1172084

Characteristics of Sea Surface Temperature During the passage of Cyclone *Phailine*.

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ABSTRACT

In Indian Ocean Bay of Bengal is the area experiencing largest number of cyclones compared to other parts, impacting property damage and human loss. *Phailine* is the cyclone that blow over Bay of Bengal and that happened on 2013 October. Sea Surface temperature has an important role in formation and intensification of cyclone. Cyclone develop only in warm water body and for which SST should be more than 26 ^{0}C. Warm water give energy for the development of Cyclone, when the water warm it make evaporation and its release latent heat and give energy to the atmosphere. We analyses changes in SST during passage of Cyclone Phailine and we found a cooling effect after the passage and strength of Cyclone is going to decrease due to cooling effect.

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DOI: https://dx.doi.org/10.5281/zenodo.1172086

Effect of B substitution on structural and magnetic properties of Zr-Co melt spun ribbons

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Abstract

Rare earth free permanent magnets have drawn much attention recently due to limited mineral resources and scarce supply of rare earth metals [1-3]. Among the rare earth free compounds, Zr_2Co_{11} is a prospective candidate that displays high uniaxial anisotropy (1.1 MJ/m^3*)* and Curie temperature (500 °C) [4, 5]. The present work focuses on investigation of effect of substitution of B in Zr-Co on structural and magnetic properties. As the phase required is stable at high temperature rapid solidification has been employed to prepare the ribbons of $Zr_{16}Co_{84-x}B_x$ (x = 0, 1,2,and 3) and the investigated the properties in both as-spun and heat-treated conditions. The x-ray diffraction (XRD) and thermo magnetic analysis revealed that substitution of B reduces the amount of soft-magnetic Co phase and increases the amount of hard-magnetic Co_2Zr_{11} phase. The addition of B in the Co–Zr melt-spun ribbons resulted in the improvement of magnetic properties, especially the coercivity. In the as-spun ribbons, with increase of B from x=0 to x=3 the coercivity increases from 0.8 to 2 KOe, while the magnetization decreases from 69 to 58 emu/g. The optimum magnetic properties of coercivity of 2.4 KOe and saturation magnetization of 77 emu/g was obtained for x=2 ribbon heat-treated at 550^{O}C for 30 min.

Key words: rare earth free magnet, $Co_{11}Zr_2$, magnetic properties

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DOI: https://dx.doi.org/10.5281/zenodo.1172092

Development of metal (Ni)/ nitride (W_2N) nanocomposite film for industrial application

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Abstract

The nanocomposite (nc) coatings have been developed very recently. These coatings show greater mechanical properties, which is mainly due to small grain sizes (10nm). The nc coatings are composed of at least two or more individual phases. A significant number of other nanocomposite coatings have also been studied. The hardness reaches a maximum when the nanocrystals of the metal nitrides are covered with one monolayer (amorphous or metallic phase). With the incorporation of metallic phase, it can give the high harness and it also gives the high toughness. Therefore, in this work W_2N/Ni nc coatings were deposited on Si (100) substrate, using DC/RF reactive magnetron Co-sputtering by varying the Ni power (0W-50W). Well-grown structures were observed in FESEM images of *nc*-W_2NN/i coating. The mechanical property of these films improves with Ni power up to 10W The best hardness (35.64 GPa), elastic modulus (250.46 Gpa) was achieved at 10W Ni target power.

Fig: shows the nanocomposite structure of W_2N/Ni and its inset show the EDAX spectra which confirm the presence of W& Ni.

Keywords: Thin film, Nanocomposite, Hardness, magnetron sputtering.

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DOI: https://dx.doi.org/10.5281/zenodo.1172096

Green Synthesis of Fluorescent Carbon Nanodots from Rose Periwinkle (*Catharanthus Roseus)* for Biosensing Applications

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Abstract

In the emerging materials research for technology and applications, fluorescent carbon nanodots (FCNDs) are a new class of carbon nanomaterials and have demonstrated fascinating optical properties for bioimaging and biosensing applications. Here we report, a green synthesis of FCNDs using rose periwinkle (*Catharanthus roseus)*flowers which are plucked from the departmental garden. The as-prepared FCNDs are characterized by X-ray diffraction, transmission electron microscopy, Fourier transform infrared (FTIR), UV-Vis absorption and fluorescence spectroscopy techniques. The fairly good fluorescent property of the prepared FCNDs is applied for biosensing applications. The calculated regression coefficient and limit of detection show that the prepared FCNDs are highly sensitive for biosensing applications.

Keywords: Carbon nanodots; Fluorescence property; Biosensing

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Synthesis of carbon dots from rose periwinkle flower using pulsed laser ablation for white light photocatalysis.

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Abstract:

In this work, we have successfully developed a facile and green synthesis of Carbon quantum dots (CQDs) from naturally available Nithyakalyani flower (Rose periwinkle) extract as a precursor using one-steppulsed laser ablation method (1). As synthesized CQDs were characterized by X Ray Diffraction(XRD), UV-Visible spectroscopy, Photoluminescence(PL), Raman Spectroscopy, Fourier transform infrared spectroscopic(FTIR) technique and Transmission electron microscopy(TEM) techniques. Moreover, we have demonstrated that the prepared CQDs could serve as an excellent photocatalyst towards the degradation of the Methylene Blue (MB) dye under white light radiation. The degradation mechanism of MB dye could be approximated as pseudo - first order kinetics according to the Langmuir – Hinshelwood model (2).

Keywords: Rose periwinkle, Carbon quantum dots, catalyst, photocatalysis.

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DOI: https://dx.doi.org/10.5281/zenodo.1172104

Structural and mechanical properties of sputtered W_2N-Ti multilayer thin films

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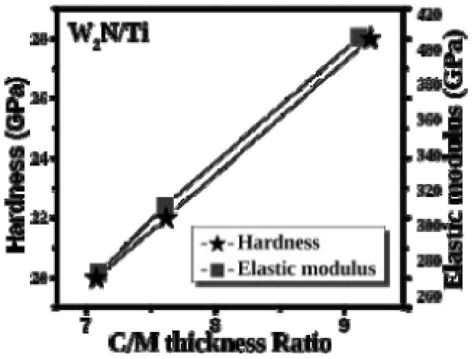
Abstract

Protection of materials by applying hard coatings over it is one of the important and versatile means of improving component performance by reducing friction, increasing wear resistance and increasing its life.Multilayer coatings with combination (10BL, 20BL & 30BL) of transition-metal nitride (tungsten nitride, W_2N) and ductile interlayers (Ti) were deposited by reactive DC magnetron sputtering technique on silicon substrates. Structural and Mechanical properties of the deposited samples were analyzed by GIXRD, FESEM, EDX and nanoindentation tests. GIXRD result confirms the presence of cubic W_2N phase. FESEM image shows periodic arrangement of W_2N and Ti. Mechanical parameters like hardness, elastic modulus & resistance to plastic deformation were calculated. The effect of different factors e.g. ceramic/ metal (C/M) ratio, interlayer material and interface on mechanical properties were discussed. These results indicate that these factors play a dominant role in defining mechanical properties. The best mechanical properties was observed for 20 BL in comparison with 10BL and 30BL coating and has been attributed to higher ceramic to metal thickness ratio.

Keywords: Multilayer; Hard Coating; Hardness; Sputtering; nanoindentation,



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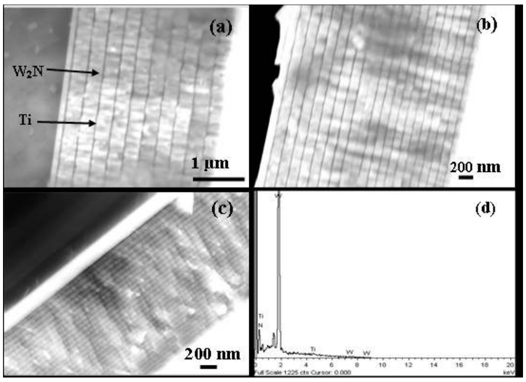

Figure: (a) Cross-sectional FESEM & EDAX and (b) Hardness Vs Ceramic/Metal ratio of W_2N/Ti multilayer.

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DOI: https://dx.doi.org/10.5281/zenodo.1172106

A Crossover from First order transition to Second Order transition in $Nd_{1-x}Cd_xMnO_3$ (x = 0.2, 0.3): Critical Behavior Study

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The magnetic and transport properties of perovskite manganties are controlled by bandwidth, which can be modified by the internal (doping) pressure at A-site, and therefore, first order transition to second order transition and/or vice versa through internal (doping) pressure is achievable. Generally, second order phase transitions are characterized by three well-defined constants termed as critical exponents, and These are encompassed by four types of universality models such as: the mean field, 3D Heisenberg, Tricritical mean field and 3D-Ising. Here, we report the doping effect of divalent cation Cd^{2+} at Nd-site of $NdMnO_3$ by magnetization measurements. $Nd_{1-x}Cd_xMnO_3$ (0.2) samples exhibits first order nature, whereas $Nd_{1-x}Cd_xMnO_3$ (x = 0.3) samples exhibit second order nature. It confirms a crossover from first order transition to second order transition while $x = 0.2$ to $x = 0.3$. The critical exponents are estimated of $x = 0.3$ sample has been analyzed using Arrott and Kouvel-Fisher plots. and the corresponding values are $\beta = 0.5176$, $\gamma = 1.0816$, $\delta = 3.45$ with $T_C = 85$ K. The estimated critical exponents of these samples are matched with mean free model, which can be explained by the existence of dipole-dipole interaction by the Cd doping which strengthens long range FM interactions between the spins. Hence, $Nd_{0.8}Cd_{0.2}MnO_3$ and $Nd_{0.7}Cd_{0.3}MnO_3$ may be very good potential candidate for refrigeration technology.

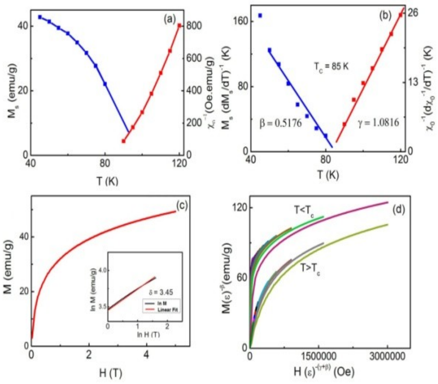

FIG. (a) M_s and χ_0^{-1} of $Nd_{0.7}Cd_{0.3}MnO_3$; (b) Kouvel-Fisher Plots for $Nd_{0.7}Cd_{0.3}MnO_3$; (c) M *vs* H at $T = T_C$ for $Nd_{0.7}Cd_{0.3}MnO_3$ [inset shows $\ln M$ *vs* $\ln H$ for δ]; (d) scaling plot below and above T_C for $Nd_{0.7}Cd_{0.3}MnO_3$.

DOI: https://dx.doi.org/10.5281/zenodo.1172111

Metal Assisted Chemical Etching of porous silicon for Photo Voltaic Application

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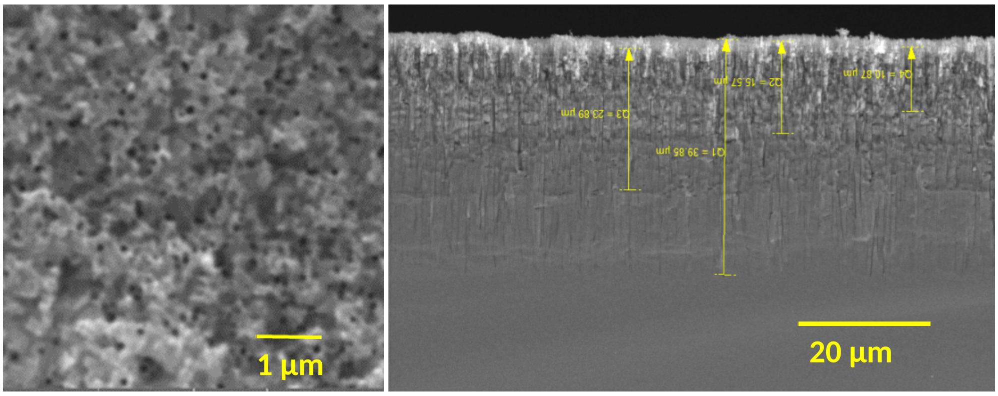
Recently, metal-assisted chemical etching (MACE) has been proposed as a promisingmethod for the fabrication of porous silicon. Here we report on MACE ofCz-Silicon by varying the etching timefor a constant silver nanoparticles (~80 nm) as the catalyst.Porous silicon (PSI) layer properties such as porosity, thickness and depth of the pores were determined.The surface morphology was examined using scanning electron microscopy, the cross sectional SEMimage on PSI revels the depth of the pore and their characteristic feature. The optical properties of the porous silicon layers were examined by diffused reflectance method. The observed results was discussed with respect to different etching time. The various experimental aspects intervening in manufacture and the characterization of the thin layers of porous silicon for photovoltaic application were studied.

Keywords: MACE, porous silicon, etching time and SEM



DOI: https://dx.doi.org/10.5281/zenodo.1172115

Impact of Copper(II) chloride in Barium titanate on its structural and optical properties

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Abstract

Copper (II) chloride is doped with barium titanate ($BaTiO_3$) for different weight percentage by sol-gel and hydrothermal method. The impact of doping copper (II) chloride on the structuraland optical properties of $BaTiO_3$ is studied. XRD revealstetragonal phase structure of $BaTiO_3$ nanopowder with traceable amount of impurities. Copper (II) doped $BaTiO_3$ nanopowder possess distorted tetragonal symmetry which is determined by the changes observed in its c/a ratio. SEM and TEM images confirms change in the morphology with the increase in the dopantconcentration. UV-Vis absorption spectrum and PL spectrum exhibits the characteristic peak of $BaTiO_3$ for all the samples and exhibits blue shift on the addition of copper (II). The FTIR spectrum provides the details on the functional group and frequency modes of Raman spectrum confirms the presence of tetragonal symmetry for undoped $BaTiO_3$ and distorted tetragonal phase for copper (II) doped $BaTiO_3$. The non-linear optical properties were compared for the doped and undoped barium titanate nanopowder.

DOI: https://dx.doi.org/10.5281/zenodo.1172125

Growth aspects of 4-Dimethylamino-*N*-methyl Stilbazolium Tosylate (DAST) organic single crystals

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Abstract

To obtain large SHG efficiencies, the organic ionic salt crystal 4-Dimethylamino-*N*-Methyl Stilbazolium Tosylate (DAST) was synthesized and characterized using proton NMR, powdered XRD and elemental analysis. Moreover, DAST seed crystals have grown from solution using a variety of solvents with three different way of synthesis. The solvents were chosen namely allyl alcohol, acetonitrile and methanol. Among these, methanol and acetonitrile are preferred as best solvents. Albeit lot of difficulties were faced to avoid or control the hydration because DAST has the tendency to form as DAST.H_2O and in which influence the symmetry also. DAST crystallizes as both centro-symmetric and non-centro-symmetric nature depends upon the solvent used. The grown crystals where appeared as dark green and orange-red colour and they were also subjected to FTIR, NMR, PXRD, SXRD for confirmation studies. From Powder XRD hydrated peak has acquired. Subsequently, repeated action has taken to rectify the hydrous form of DAST. Moreover correlation was found at hydrous peak acquired at NMR, FTIR and PXRD. During growth suitable oil is sprayed at the surface to reduce this hydration.

DOI: https://dx.doi.org/10.5281/zenodo.1172127

Functional Materials for Environmental Remediation

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Fenton catalysts (H_2O_2/Fe^{2+}) are employed for environmental remediation through the Fenton mechanism involving reactive oxygen species (ROS). Storage and transportation of H_2O_2 limits its applications. ROS mediatedoxidation process involved in Fenton process and semi-conductor based photo catalysis, is attributed for dye degradation and antimicrobial applications in waste water Usually in latter process, semiconductor photocatalysts such as TiO_2andZnO are being used, as these generate ROS through redox reactions of holes and electrons generated in aqueous suspensionsdue to absorption of light.However, there is a need for development of a catalyst that generates ROS even in absence of light so that the applications are enhanced.

In this talk, our successful efforts in the design and development of such a new catalyst.ZnO_2/Polypyrrole.that generates ROS even in absence of light through synergy and its application in dye degradationwill be illustrated [1]. It is to be noted that neither ZnO_2 nor Polypyrrole degrades dyes in presence or absence of visible light. Furthermore, the rate of dye degradation of our nanocomposite is higher than that of the commercial catalyst.

We have also linkedphotocatalytic reaction to Fenton reactionin the catalyst ZnO_2/Fe^{2+} that could have potential applications, as it employs solid oxidant ZnO_2 in place of less stable H_2O_2 [2].

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DOI: https://dx.doi.org/10.5281/zenodo.1172133

Effect of hydrostatic pressure on superconducting properties and flux dynamics of Fe and Cr substituted $NbSe_2$ single crystal

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Abstracts:

Magnetization measurements have been used to determine the effect of magnetic impurities (Fe and Cr) on the Larkin–Ovchinnikov (LO) 3D collective pinning model in $NbSe_2$ single crystals under the hydrostatic pressure (P) up to 1 GPa [1,2]. We found that the pressure can induce a transition from the regime where pinning is controlled by spatial variation in the critical transition temperature (δT_c) to the regime controlled by spatial variation in the mean free path ($\delta\ell$) [3]. Furthermore, T_c and low field J_c are slightly induced, although the J_c drops more rapidly at high fields than at ambient P. The pressure effect enhances the anisotropy and reduces the coherence length, resulting in weak interaction of the vortex cores with the pinning centers. Moreover, the P can induce the density of states, which, in turn, leads to enhance in T_c with increasing P. The intrinsic disorder in pure $NbSe_2$ single crystals shows δT_c flux pinning; however, the extrinsic disorder created by doping atoms in $NbSe_2$ shows $\delta\ell$ flux pinning and application of P. Both $\delta\ell$ and δT_c core pinning strongly enhance the coupling between the vortices in the randomized pinning potential, which makes the 3D magnetic fluxes into 2D nature. P enhances the T_c with the rates of dT_c/dP is higher compared to the ambient. The magnetization data are used to establish a vortex phase diagram. The nature of the vortices has been determined from the scaling behaviour of the pinning force density extracted from the J_c–H isotherms and demonstrates the point pinning mechanism.

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DOI: https://dx.doi.org/10.5281/zenodo.1172135

Investigation on Magnetic Structure for transition metal difluorides of NiF_2

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NiF_2 is one of the interesting candidates from the family of complex non-oxide functional materials namely transition metal (TM) fluorides (MF_2 (M = Ni, Fe, Mn, Co). Its exotic properties are advantageous towards electric and magnetic applications. The tetragonal unit cell consists of two formula units with two M atoms in the unit cell, one at corner of the cell and another at body diagonal position. The Ni^{2+} ions at the corners and body centers of the unit cell forming two opposed sub lattice with the spins along the *c*- axis and the spins are tilted away from *c*- axis by ~10 degrees. Its tetragonal structure which goes below T_N =71.3 K in to AFM state with week FM state. *Paul A Fleury (1969)* reported the observation of magnetic light scattering in NiF_2 in both its anti-ferromagnetic and paramagnetic phase. The refined structure of NiF_2 is tetragonal structure which belongs to rutile type crystal structure. This study explore that NiF_2 exhibit anti-ferromagnetic phase at the transition point if T_N=68.5 K and weak ferromagnetic transition occurs below that temperature. This present results enrich the understanding of the structural and magnetic behaviour of NiF_2 transition metal difluoride.

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DOI: https://dx.doi.org/10.5281/zenodo.1179397

Potential and indispensable high temperature superconductivity in novel Rare Earth Hydrides under higher pressure.

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Abstract

Room-temperature superconductivity has been a long-held dream and an area of intensive research. Recently, Rare earth hydrides have demonstrated the potential for achieving room temperature superconductivity under high pressure which changes the density of states at the Fermi level, electron-phonon coupling. The proposed project consists of synthesis and characterization of new REH_{12-x} [RE= La to Yb] Rare Earth Hydrides in which H atoms are weakly covalently bonded to one another, with rare earth atoms occupying the centers of the cages(H clathrate structures)The clathrate structures exhibit potential high-T_c superconductivity that originates from the large H-derived electron density of states at the Fermi level and the strong electron-phonon coupling which is related to the motion of H atoms within the cages. The profound implications will be stated after an introduction of Rare Earth Hydrides. Additionally theoretical predictions and subsequent experimental observations of high-temperature superconductivity in dense hydrogen-rich compounds will be reviewed.

In Experimental techniques, PPMS-VSM (9T-QD, USA)and Closed Cycle Refrigerator -variable temperature insert (CCR-VTI) and hybrid piston-cylinder pressure cell (~3.5 GPa), Modified Bridgman anvilpressure cell (~ 8 GPa-MB-cell) and Diamond anvil pressure cell (DAC) upto 50 GPa suitable withCCR-VTI, 1.5 GPa pressure Cell suitable for M(T) and M(H) measurements, at low temperature (2 K)and magnetic field (9 T) will be discussed.

Our work will stimulate future high-pressure experimental work on synthesis of these Rare Earth Hydrides with clathrate structures to explore the high-Tc superconductivity and the peculiar

DOI: https://dx.doi.org/10.5281/zenodo.1179399

chemical bondings involved.The results open the prospect for the design, and recovery of new high temperature superconductors with potential practical applications.

DOI: https://dx.doi.org/10.5281/zenodo.1179399

Synthesis and Temperature induced Structural Phase Transition in Schiff Base Soft Materials

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Research Abstract

The purpose of the research work is to examine whether structural modification through phase transition might result in detection of new potential materials having thermal storage capacity, linear optical property and thermochromic property to achieve the device performance. New phase transition materials with loosely bound systems of Schiff based soft materials will be developed. A series of experiments to the intermolecular hydrogen bonded Systems with required characteristics will be designed. The various characterization techniques such as Neutron diffraction studies, Single X-ray diffraction, Powder X- ray diffraction with phase transition studies, Differential scanning calorimetry with specific heat capacity (Enthalpy, Entropy) and Vickers hardness with elastic constants, will be done and observed the changes in the physical and chemical properties of the synthesized materials, more potent than the standard one. We hope that the structural modification lead to uniform alteration in all physical and chemical activity and useful in the device performance.

DOI: https://dx.doi.org/10.5281/zenodo.1179451

Semiconductor to metallic transition of $Ba_2BiFeSe_5$ under external pressure

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Abstract:

Low-dimensional transition metal chalcogenides have attracted much attention in material science, solid state chemistry, and crystal engineering. This is because these compounds are the potential targets to explore the interesting physical properties caused by the quantum many-body effects [1] and potential applications, including thermoelectrical [2] nonlinear optical (NLO) [3] electronic phenomena, and unusual magnetic properties [4] In particular, one-dimensional Heisenberg antiferromagnetic (1D HAF) chain compounds have still been a hot topic. Since Haldane's theoretical prediction, which was made in 1983 [5]. Here, the structure of $Ba_2BiFeSe_5$ is built from distorted FeSe4 tetrahedra and BiSe5 quadrangular pyramids, which are connected to each other in an alternating fashion to generate the infinitely corrugated quasi-1D $[FeBiSe5]_{\infty}$ anionic ladders. It exhibits a paramagnetic (PM) to canted antiferromagnetic (C-AFM) transition achieved by means of competing super-exchange interactions [10]. The temperature dependence of resistivity ρ(T) demonstrates the semiconducting property of this sample. The suppression of semiconducting behavior and its lead to induced metallic nature with application pressure up to 12 GPa. The low temperature resistivity curve suppresses and induced metallic nature is observed from the activation energy E_a was estimated to be 0.168 eV by the Arrhenius equation, $\rho(T)=\rho_0 \exp^{(Ea/kBT)}$, The observed activation energy (*Ea*) is 0.168 eV (0 GPa) to 0.006 eV (12.3 GPa). The strong suppression of the semiconducting behavior in $Ba_2BiFeSe_5$ suggests that the Fermi surface is in the vicinity of some instability. It is plausible that the Fermi level is located near the edge of the conduction band. This indicates that induced superconductivity is realized in the complex Fermi surface including the impurity band with a low carrier density and a low density of states, and it rather provides benefit for achieving a higher T_c with application of higher pressure.

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DOI: https://dx.doi.org/10.5281/zenodo.1182353

Investigation on transport properties under extreme conditions of hydrostatic pressure and magnetic field on $Nd_{1-x}Cd_xMnO_3$ ($x = 0.4$)

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Abstract:

We investigate the temperature dependence of the electrical resistivity and field dependence of magneto resistance of $Nd_{1-x}Cd_xMnO_3$ ($x = 0.4$) perovskite manganites. Figure 1 (a) and (b) show that electrical resistivity measurements in the temperature range 50 – 300 K at ambient pressure and 1 GPa hydrostatic pressure respectively which indicate metal- insulator transition at 90 K and 97 K in the cooling cycles and 107 K and 115 K in the warming cycles at ambient pressure and 1 GPa hydrostatic pressure respectively. When the pressure increases at 1 GPa, the metal-insulator transition (T_{MI}) temperature which shift to higher temperature. We investigate that the magneto resistance (MR) of the material in the temperature interval ΔT = 5K at magnetic field (-5T to +5T) under ambient and hydrostatic pressure 1GPa. The negative magneto resistance has decreased by applying pressure at 1GPa. Pressure increases the T_{MI} metal-insulator transition temperature and decrease the negative magneto resistance value.

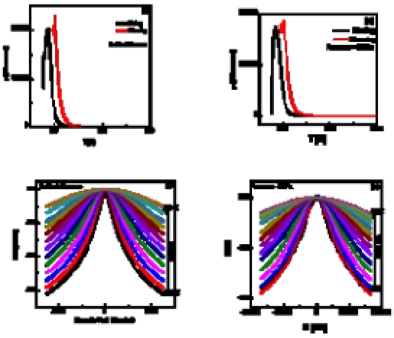

FIG. 1. (a) and (b) Temperature dependence resistivity of $Nd_{1-x}Cd_xMnO_3$ ($x = 0.4$) at ambient and 1GPa hydrostatic pressure respectively, (c) and (d) field dependence of magneto resistance (MR) of $Nd_{1-x}Cd_xMnO_3$ ($x = 0.4$) in the temperature interval ΔT = 5K at magnetic field (-5T to +5T) under ambient and hydrostatic pressure 1GPa respectively.

DOI: https://dx.doi.org/10.5281/zenodo.1182368

Effect of Plant Mediated Synthesis on Structural, Electrical, Optical and Anti-bacterial Studies of Zinc Oxide Nanoparticles

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Plant mediated synthesis has been suggested as easy, low cost and eco- friendly method [1]. Zinc oxide nanoparticles (ZnO 1 , ZnO 2 , ZnO 3) were synthesized by plant mediated synthesis using the medicinal plants, Andrographis paniculata, Phyllanthus niruri and Carica papaya. The hexagonal wurtzite structure of all the three ZnO NPs was confirmed by XRD. SEM analysis shows variations in morphology for ZnO 1, ZnO 2 and ZnO 3. The alterations in absorption and bandgap and dielectric constant are due to the reaction rate of phytochemicals during synthesis besides size effects. All the three nanoparticles produce high excitonic UV emission in addition to blue light emission. Two gram positive bacteria such as Staphylococcus aureus and Bacillus subtilis and two gram negative bacteria such as Pseudomonas aeruginosa and Escherichia coli were taken for antibacterial study. The order of antibacterial activity for S.aureus is ZnO 1 > ZnO 3 > ZnO 2 and for B.subtilis is ZnO 3 > ZnO 1 > ZnO 2. The activity of ZnO 3 is 10% less than ZnO 1 and ZnO 2 for P.aeruginosa and ZnO 1 and ZnO 3 is 5% less than ZnO 2 for E.coli. The very high surface to volume ratio as well as the release of reactive oxygen species of ZnO nanoparticles gives rise to high toxicity to micro organisms thereby leading to large zone of inhibition [2, 3].

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Enhanced superconductivity in Se-doped $EuSr_2Bi_2S_4F_4$ and $Eu_2SrBi_2S_4F_4$ under hydrostatic pressure

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Abstract:

The recently known BiS_2 layer containing superconductors has gained considerable attention. After the discovery of superconductivity in layered $Bi_4O_4S_3$ compounds has a tremendous amount of work on comes on BiS2-based systems has been carried out in the past six years. Here, the modification of superconductivity in the parent compound could be of great importance in studying both mechanism of superconductivity and exploration of new SC compounds at ambient and high-pressure conditions. Recently, we reported the induce superconductivity in $EuSr_2Bi_2S_4F_4$ by Se substitution at the S site (isovalent substitution) with T_c of ~ 2.9 K in $EuSr_2Bi_2S_2Se_2F_4$. The other compound, $Eu_2SrBi_2S_4F_4$, shows a significant enhancement of T_c. In Se-substituted $Eu_2SrBi_2S_{4-x}Se_xF_4$. At the same time, superconducting T_c of ~ 2.6 K for x = 1.5 and T_c of ~ 2.8 K for x = 2, whereas T_c of ~ 0.4 K in the Se-free sample. The enhancement of superconductivity in an important effect associated with Se substitution is that it gives rise to remarkable changes in the Eu valence. Further, here we report a systematic investigation of Se substituted in $Eu_2SrBi_2S_{4-x}Se_xF_4$ and $EuSr_2Bi_2S_{4-x}Se_xF_4$(x=1.5 and 2) by electrical resistivity and magnetic susceptibility measurements under various applied pressures ranging from 0 to 3 GPa. Surprisingly, on applying external pressure we observe enhanced superconductivity in all the materials. Particularly, Highest Tc observed in $EuSr_2Bi_2S_2Se_2F_4$ compound at ~ 8 K (3 GPa) with 1.68 K/GPa. The field dependent upper critical field (H_{c2}) and thermal activation energy (U_0) was calculated using Werthamer–Helfand–Hohenberg (WHH) equation. The thermal activation energy of charge carriers could be determined from the thermal activation formula. The important essential properties of all the compounds are analyzed with application magnetic field and high pressure.

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DOI: https://dx.doi.org/10.5281/zenodo.1182399

Generation of Terahertz Frequencies Using Potentially NLO active Organic High Quality Single Crystals of BNA and DAST - An Indigenous Approach

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Abstract

The field of generation and detection of Terahertz (THz) frequencies has attracted worldwide attention since many important molecules such as proteins, pharmaceuticals, explosives, narcotic drugs, etc., exhibit their characteristic fingerprints in this region of the electromagnetic spectrum [1]. However, developing proper sources and detectors in this region has been a serious problem and attempts are being made to narrow down the gap between the optic and electronic region which is known as “THz gap” in the electromagnetic spectrum [2-3]. In coming decades, a lot more innovative research is expected in this area and the continuing effort to identify more compact, powerful sources in THz range. In this direction, BNA and DAST material (NLO coefficient of 234 and 1100 pm/V respectively) has been synthesized and high-quality twin free single crystals were grown by slow evaporation solution technique. The grown single crystals were potentially used to generate THz waves in the frequency range (0.2-3 THz).

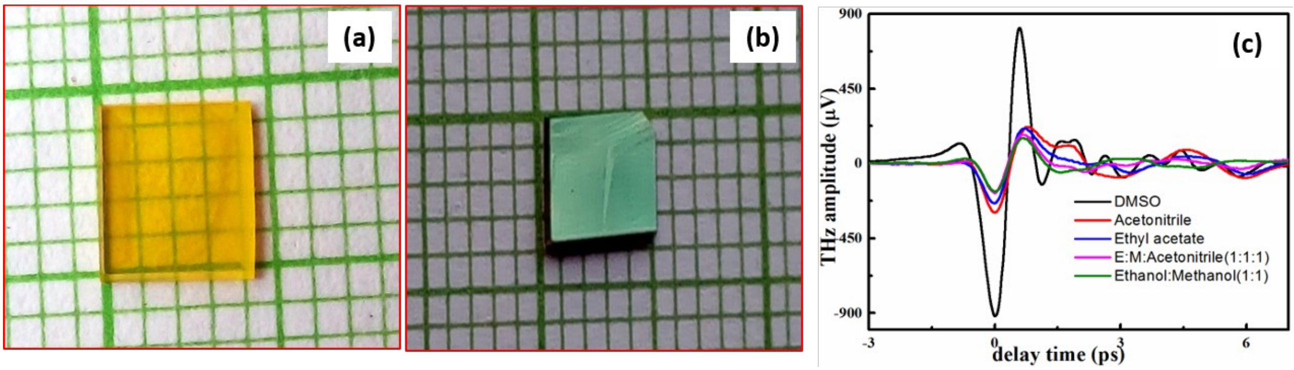

Figure 1. Photograph of indigenously grown (a)BNA and (b) DAST Single crystals (c) Amplitude spectra of THz waves generated from BNA single crystals of various solvents.

Keywords: Organic Materials, Crystal Growth, Terahertz Generation and Detection

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DOI: https://dx.doi.org/10.5281/zenodo.1182401

Pressure-Induced Quantum Phase Transition in Boron Doped Diamond Thin Film

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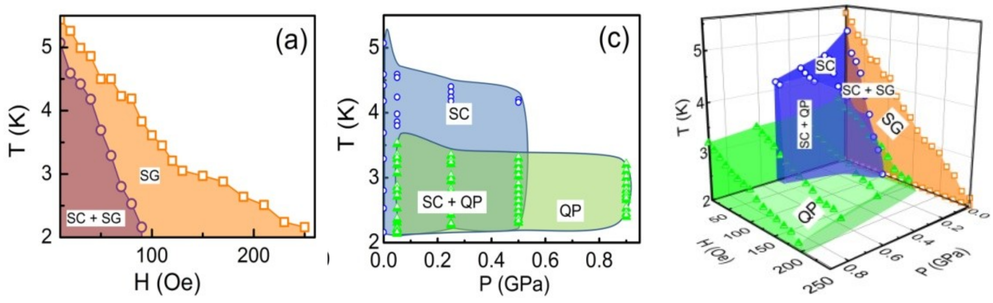
Diamond in the form of thin films possess negative electron affinity characteristics. Hence, it is one of the important elements for electronic applications such as microchip substrates, high-efficiency electron emitters, photodetectors, transistors etc [1]. Boron has the smaller atomic radius and has one less electron than the diamond.

By the increasing of boron in pure diamond film, a semiconductor - metallic - superconducting transition is observed at the various concentrations such as of 0.3×10^{21} , 0.5×10^{21} and 0.6×10^{21} cm^{-3} [2]. Moreover, the presence of one free electron-boron impurity in boron doped diamond may induce a kind of smallest scale energy, quantum level change. Here, we have investigated the magnetic property of high concentrated (2.9 x 10^{21} cm^{-3}) Boron doped Diamond under very low perturbations such as temperature region (10 to 2 K), pressure (up to ~1 GPa), magnetic field (up to 6000 Oe). The application of a small pressure of 0.05 GPa at 10 Oe introduces a new anomaly near the very low temperature, and it is termed as Quantum Phase Transition. While increasing of magnetic field under different pressures such as 0.05 GPa, 0.25, 0.5 and 0.9 GPa, the QPT is continued to exist till 110 Oe, 130 Oe, 140 Oe and 150 Oe respectively. *i.e.*, the pressure supports to enhance the QPT transition. By having these complete information, two dimensional phase diagrams (H-T), (P-T) and a three dimensional (*P*-*H*-*T*) phase diagram for BDD of our concentration is reported for the first time as shown in figure 3.



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DOI: https://dx.doi.org/10.5281/zenodo.1182405

Proceedings Of 29th Annual General Meeting Of Materials Research Society Of India And National Symposium On Advances In Functional And Exotic Materials

Hydrostatic Pressure Effect on martensite transition and Magnetocaloric Properties of $Ni_{1.75}Pt_{0.25}MnGa$ Heusler alloy.

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Abstract:

The effect of hydrostatic pressure on the magnetic and Magnetocaloric properties of $Ni_{1.75}Pt_{0.25}MnGa$ shape memory Heusler alloy around the martensitic transition has been investigated. We find that the application of hydrostatic Pressure increases the martensitic transition temperature (T_M) for $Ni_{1.75}Pt_{0.25}MnGa$ by $dT_M/dP = +3.89$ K/GPa and therefore pressure stabilizes the martensite phase. This phenomenon could be accounted for as follows. Increase of pressure would reduce the unit cell volume, which influences T_M and other characteristic transition temperatures. With increasing pressure from 0.32GPa to 0.95Gpa blocking temperature is shifted from 200 K to 250K. The maximum magnetic entropy change (ΔS_{max}) is found to be reduced from 9.29 J Kg^{-1} K^{-1} to 5.48 J Kg^{-1} K^{-1}around $\mathbf{T_M}$ for $Ni_{1.75}Pt_{0.25}MnGa$ and RCP increases linearly with the application of field upto 0.91GPa but the maximum RCP decreases with the application of pressure upto 9 GPa. Magneto crystalline anisotropy possibly arises due to the volume change by increase in hydrostatic pressure.

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