

NPL – RSC Symposium on Advanced Nanomaterials for Energy

Event Programme

Time	Speakers	Title
9:00-9:15 am	Registration	
9:15-9:25 am	Dr. D.K. Aswal, Director National Physical Laboratory, New Delhi	Opening remarks
9:25-9:45 am	Dr. Ashok K. Chauhan, Founder President, Amity University	Inaugural Talk
09:45-10:15 am	Professor Neil Champness, University of Nottingham, UK	Molecular Organisation: Working with Molecules on the Nanoscale
10:15-10:45 am	Dr. R.K. Kotnala, National Physical Laboratory, New Delhi	Green Electrical Energy Device for Masses Runs on Water only - Hydroelectric Cell
10:45 -11:15 am	Tea break	
11:15-11:45 am	Dr. S R Dhakate, National Physical Laboratory, New Delhi	Application of non-materials for renewable energy: Indian Perspective
11:45-12:15 pm	Dr Thomas Chamberlain, University of Leeds, UK	Stabilised Metal Nanoparticles in Tailor-made Carbon Nanoreactors as Tuneable Heterogeneous Catalysts for Continuous-flow Processing
12:15-12:45 pm	Dr. D. Haranath National Physical Laboratory, New Delhi	Nanophosphors for efficient energy
12:45-1:15 pm	Flash presentations	8- Speakers
1:15-2:30 pm	Lunch/Posters	
2:30-3:00 pm	Dr Graham Newton, University of Nottingham	New Approaches to Molecular Metal Oxide Photoactivation
3:00-3:30 pm	Dr S M Shivaprasad, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore	Some Exotic Properties of the GaN Nanowall Network
3:30-4:15 pm	Dr Deeksha Gupta, Royal Society of Chemistry	How to publish in high impact journals
4:15-5:00 pm	Poster Presentation/tea	
5:00 pm	Concluding and Prize distribution	

Supramolecular Nanostructure Fabrication

Neil Champness
The University of Nottingham, UK
Email: neil.champness@nottingham.ac.uk

Neil's lecture will describe his research on employing a supramolecular approach for nanostructure fabrication allowing the preparation of functionalised surface supramolecular arrays and the entrapment of complex molecular species. Internationally recognised highlights include the demonstration of hydrogen-bonded templates [*Nature* **424**, 1029 (2003)], random molecular tilings [*Science* **322**, 1027 (2008); *Nature Chem.* **4**, 112 (2012)], guest-induced supramolecular networks [*Nature Chem.* **3**, 74 (2011)] and sub-molecular imaging of hydrogen-bonded arrays using DFM [*Nature Commun.*, **5**, 3931, (2014)]. He will also describe the synthesis of metal-organic frameworks (MOFs) and their use in guest entrapment [*Nature Chem.*, **1**, 487, (2009)] and photochemical applications [*Nature Chem.* **2**, 688 (2010)].

New Approaches to Molecular Metal Oxide Photoactivation

Graham N. Newton
University of Nottingham, UK
Email: graham.newton@nottingham.ac.uk

Molecular metal oxides constructed from oxo-bridged early transition metals in their highest oxidation states, polyoxometalates (POMs) are characterised in large part by their rich redox chemistry, leading to potential applications in catalysis, nano-scale electronics and magnetism. In addition, their capacity to form highly active photo-excited states (oxo-centred radicals) upon excitation of the O→M ligand-to-metal charge transfer (LMCT) band, has led to sustained interest in their use as both heterogeneous and homogeneous photocatalysts for a range of transformations. Typically, however, the POM LMCT band is located entirely in the UV region, limiting their utility in solar driven processes.

Here, two contrasting approaches to the visible light photosensitisation of hybrid POMs will be discussed and the concepts of 'exo' and 'endo' charge-separation will be introduced.

Stabilised Metal Nanoparticles in Tailor-made Carbon Nanoreactors as Tuneable Heterogeneous Catalysts for Continuous-flow Processing

Thomas W. Chamberlain
University of Leeds, UK
Email: T.W.Chamberlain@leeds.ac.uk

Tom's research focuses on the controlled fabrication of carbon nanostructure (CNS) supported catalysts and their characterisation down at the atomic level. Using solid state analytical techniques including aberration corrected high resolution electron microscopies (AC-HRTEM and STEM), X-ray absorption and diffraction and gas adsorption it is possible to elucidate their exact structure. By monitoring both the formation of heterogeneous catalysts from metallic precursors and the structure of the catalyst during chemical reactions using a combination of in situ HRTEM and near edge X-ray absorption fine structure (NEXAFS) experiments it is possible to reveal atomic level structural information and mechanistic details about how the catalysts function. Our detailed understanding of nanomaterial formation processes has enabled a wide variety of CNS supported materials to be fabricated, including metallic and bimetallic systems, e.g. NiRu and PtRu nanoparticles, metal oxides, e.g. Fe_2O_3 and Co_3O_4 , and inorganic materials, e.g. MoS_2 , PtI_2 . It also enables different metal loadings to be achieved, as well as, control over nanoparticle size and location.

Using this understanding it has been possible to both optimise the fabrication and explore the performance of our supported materials in heterogeneous catalysis in packed bed continuous flow and electrochemical reactor systems (Figure 1).[4,5] This has enabled rapid optimisation of both reaction conditions and catalyst composition. Incorporating in-line analysis coupled to evolutionary algorithms enables rapid screening of reaction conditions and maximises yield and/or throughput.

Some Exotic Properties of the GaN Nanowall Network

S.M. Shivaprasad

International Centre for Materials Science

Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru- 560064

Email: smsprasad@jncasr.ac.in

The band-gap engineering of wide band-gap semiconductors by alloying with a iso-valent elements enable them to absorb and emit over a wide range of wavelengths from UV to IR. Combining this tunability with size induced functionality at nano-dimensions, result in multi-functionality that can be harnessed for several applications.

I shall present our experimental results of the kinetically controlled growth of self-assembled nanostructures of GaN thin films formed by Plasma Assisted- Molecular Beam Epitaxy. Among the several epitaxial nanostructures we obtain, I shall present the details of 'nanowall network' which consists of wedge shaped walls that circumscribe polygonal cavities. The epitaxial nanowalls are dislocation and strain free and possess a high density of band-tail states, making it highly conducting and luminescent. The apex of the walls and the cavity dimensions make the system suitable for both electron and optical-photon confinement, respectively. Cathodoluminescence reveals that the band-edge UV-band is spatially confined to the walls, while a novel NIR band is emitted from the voids, which at low temperature show a laser-like spontaneous emission. The morphology induced charge accumulations in nanowall apex regions is seen to result in a 2-DEG, yielding a very-high electron mobility and even magnetic ordering of the itinerant charges. We have also used this material with large surface area, decorated with Ag nanoparticles, as a substrate for Surface Enhanced Raman Spectroscopy with large enhancement factors and very low detection limits for R6G analyte. The use of this nanowall as a template for dislocation filtered GaN overlayers by lateral growth will also be shown.

Water management system by GSM using nanostructured magnesium oxide

Neeraj Marwaha and A.K. Srivastava
*Academy of Scientific & Innovative Research,
CSIR - National Physical Laboratory, New Delhi-110012, India
Email: aks@nplindia.org**

Metal oxides play a very important role in many areas of electronics, chemistry, physics, water management systems (WMS) and materials science. These can adopt a large number of structural geometries with a proper electronic structure that can exhibit metallic, semiconductor or insulator character. The Photoluminescence properties of MgO widely study both experimentally and theoretically due to presence of defects at the surface sites and their large band gap^[1,2], thus it gain significant attention among various research group in this area and become a huge research topic^[3,4]. In this prototype, we investigate the various technologies available in the market for SMS based canal pipeline water management. We motivate our research and provide a conceptual introduction which illustrates the need to increase or decrease the level of water, by activating three different water gates represented by water pumps here. If there is need to increase the level of water, we can do, decrease the level then also we can do by two different SMS. Subsequently, we suggest general system architecture for this mobile based irrigation system for different application for farmers and discuss related design decision^[7-9]. This design has been implemented as a prototype which we named "Water management system for horticulture using global service mobile (GSM) enabled and MgO nanoparticles for display".

A GSM technology is available in the market for water management system is proposed. A conceptual introduction which illustrates the need to increase or decrease the level of water by activating three different water gates represented by water pumps here. If there is need to increase the level of water we can do similarly we can decrease the level by sending two different SMS. As a first step towards a solution we take user's prospective for water saving and time management which can be deployed on the basic mobile handset device. Subsequently we suggest general system architecture for this mobile based horticulture system application for a farmer and discuss related design decision. This design has been implemented as a prototype which we named "GSM Based Water management system". Horticulture by using water management system with SMS approach helps farmer to determine how much water their Plant has been used and how long they need to run their pump or drip system for each day using the GSM based technology and mobile phone based delivery services. Wireless device has been gaining popularity in decent year. Cellular phone and other wireless device have driven demand for new wireless technology^[10-15]. The objective of this project is to develop a device that allows the user to remotely control and monitor multiple water level management for different Plants using a cellular GSM phone. This system will be a powerful and flexible tool that will offer this service at any time, by any body and anywhere without the constraints of the technologies being applied. Possible target includes climate control system, security systems, lights, anything with an electrical interface.

Key Words: MgO; Nanoparticles; Global Service Mobile(GSM);Water Management Systems;(WMS)

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Nanoparticles doped liquid crystal based storage devices for future energy applications

Jai Prakash¹ and Ashok M. Biradar²

¹*Department of Physics, Aligarh Muslim University, Aligarh – 202002*

²*CSIR – National Physical Laboratory, Dr. K. S. Krishnan Road, New Delhi -110012*

Email: jpsphysics@gmail.com

It has been appreciated that liquid crystals (LCs) are the most promising materials for display as well as non-display (optical devices based on LC) applications in modern technology. The LCs have proved their importance in various areas of science and technology such as material science, biomedical, optics, etc. Ferroelectric LCs (FLCs) are the special members of LC family and are well known for their good optical contrast, low threshold voltage, and faster electro-optical response. In recent years, The FLCs have been found applications in storage devices (or memory devices) [1, 2]. These storage devices require less electric energy for very short duration and remain in their last state for longer duration (for few days) without any power. It has also been observed that the memory effect observed in LC materials could be enhanced by doping of nano-materials in them [3, 4].

Here, we present our work based on memory effect in FLCs/nano-materials doped FLCs. The talk will demonstrate how the fascinating and emerging world of LCs and nanotechnology will affect the energy applications. The observed electrical bistable behavior led to memory application to store a virtual '0' and '1' (off and on states). The bistability remains in either state even after the power is turned off making them ideal candidates for nonvolatile memory devices. The memory effect observed lasts for a prolonged time (several days). The memory devices would have a tremendous impact on the future of information technology and electronic industry.

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TEMPLATE ASSISTED MICROWAVE SYNTHESIS OF NANO CONDUCTING POLYMER

Ghosal, Anujit;^{1,2} Iqbal, Sajid;² and Ahmad, Sharif²

¹*Department of Chemistry, School of Basic and Applied Sciences, Galgotias University, Greater Noida, U.P.*

²*Department of Chemistry, Materials Research Lab, Jamia Millia Islamia, New Delhi.*

Conducting polymers (CP) in any size regime i.e. from bulk, micro or nanostructure have many useful applications in supercapacitors, biosensors, redox indicators, light emitting diodes (LEDs), EMI shielding materials, solar cells, field effect transistor (FET), etc.¹⁻⁴ Long conjugation length, large surface area and tunable properties of these CP gives them an edge over other metal and metal oxide nanomaterials. Various methods of synthesis for nano CP like chemical, photochemical, plasma, organometallic cross-coupling reactions, enzyme-catalyzed and electrochemical oxidative polymerization, etc, have been reported. However, the synthesis of CP with controlled morphology and size became a challenge for chemists and materials scientists. Here, we report a template assisted microwave synthesis of poly 1-naphthylamine (NPA). The conducting polymer nanostructures have been characterized using FT-IR, UV-visible, SEM analysis. These CP's can further be utilized for electrochemical corrosion inhibition application.^{5, 6}

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Study of effective charge transfer interactions in fullerene grafted graphene oxide

Rachana Kumar, Saba Khan, Chhavi Sharma, Mahesh Kumar, Pramod Kumar,
Jaishree Bharadwaj

We have covalently grafted fullerene molecules to graphene oxide using hydrolyzed PC61BM as fullerene precursor via very mild process without the use of metal catalysts and comprehensively studied the charge transfer interactions in ground and excited state. For the evidence of covalent grafting of fullerene on graphene oxide sheets different spectroscopic studies have been performed like, FTIR, Raman spectroscopy, UV-vis absorption, cyclic voltammetry and XRD. Amount of loading of fullerene on graphene oxide is calculated by thermogravimetric analysis. Covalently attached fullerene molecules act as excellent electron acceptor for ultrafast electron transfer from graphene oxide sheets and established by photoluminescence and ultrafast pump-probe transient absorption (TA) spectroscopy. From the TA measurements, we reveal ultrafast charge separation and long lived charge separated species formation in fullerene functionalized graphene oxide.

New Insight into Lanthanide doped Nanophosphor as a Broad Spectral converter (UV-IR) for Promising Next Generation Si-Solar Cell

Pawan Kumar, Amit Kumar Gangwar, Kanika, Satbir Singh and Bipin Kumar Gupta

Herein, we have successfully demonstrate the synthesis of highly luminescent downshift (DS) and upconversion (UC) $\text{Gd}_2(\text{MoO}_4)_3:\text{RE}^{3+}$ (RE=Eu, Tb, Tm, Er, Yb) nanophosphors by facile solid state reaction which can be scale up in pilot plant. The gross structural, surface morphology and microstructural characterizations of these nanophosphors have been investigated by X-ray powder diffraction (XRD), scanning electron microscopy (SEM) and transmission/high-resolution transmission electron microscopy (TEM/HRTEM) techniques, respectively. Photoluminescence (PL) and time-resolved photoluminescence (TRPL) spectroscopic methods have been used to explore the striking luminescence properties of the synthesized nanophosphors. The as-synthesized luminescent DS $\text{Gd}_2(\text{MoO}_4)_3:\text{Eu}^{3+}$ nanophosphor exhibits excitations at 291, 362, 377, 385, 416, and 465 nm with strong red emission peaking at 616 nm. The as-synthesized luminescent DS $\text{Gd}_2(\text{MoO}_4)_3:\text{Tb}^{3+}$ and $\text{Gd}_2(\text{MoO}_4)_3:\text{Tm}^{3+}$ nanophosphors exhibit a strong green emission at 541 nm and a deep blue emission at 453 nm upon an excitation wavelength of 378 nm and 266 nm, respectively. The as-synthesized luminescent UC $\text{Gd}_2(\text{MoO}_4)_3:\text{Er}^{3+}, \text{Yb}^{3+}$ nanophosphor exhibits excitations at 980 and 1550 nm with emission peaks at 542, 977, 1223 and 1328 nm. The obtained photoluminescent results suggest the full utility of $\text{Gd}_2(\text{MoO}_4)_3:\text{RE}^{3+}$ (RE=Eu, Tb, Tm, Er, Yb) nanophosphor act as a broad spectral converter (UV-IR) for promising next generation Si-Solar Cell.

Efficient energy/ charge transfer in femtosecond time domain

CHHAVI SHARMA

*Advance Materials and Devices Division, National Physical Laboratory, Dr. K.S.
Krishnan Road, New Delhi 110012, India*

Here we report two different studies revealing new charge transfer (CT) state in one and plasmon resonance energy transfer (PRET) mechanism in another. These studies have been substantiated by ultrafast transient absorption spectroscopy (TAS). In first study, we report the electric field induced polarization and the formation of a charge transfer (CT) state in the conjugated polymer. Its TAS studies have revealed an evolution of a CT state at about 772 nm in the excited state absorption (ESA) region, which is not present in the un-polarized polymer. However, the second work defines the consequences of the nanoparticle overloading amount and energy transfer process between gold nanorods and polymer (active matrix) in organic solar cells. This analysis reveals the plasmon resonance energy transfer (PRET) mechanism which enhanced the carrier population density in polymer via non-radiative process beyond the concurrence of a particular plasmon resonance oscillation mode and polymer absorption range. Hence, this work explores two ways i.e, polarization of conjugated polymers in organic solar cells at the surface and the inclusion of plasmonic nanoparticles into organic solar cell at the interface which enhances the light harvesting properties that lead to higher power conversion efficiency without altering the device configuration.

Exploration of the interaction between noscapine drug and human serum albumin

Neha Maurya, Meena Kumari, Jitendra Kumar Maurya, Upendra Kumar Singh, and Rajan Patel*

Biophysical Chemistry Laboratory, Centre for Interdisciplinary Research in Basic Sciences, Jamia Millia Islamia (A Central University), New Delhi-110025, India.

Tel.: +91 8860634100; fax: +91 11 26983409.

Email: rpatel@jmi.ac.in, rajanpatel@jmi.ac.in (Dr. R. Patel)

Noscapine is a phthalideisoquinoline alkaloid extracted from plant, *Papaver somniferum* with efficiency to inhibit cellular proliferation and induced apoptosis in non-small cell, lung, breast, lymphoma and prostate cancer. In this prospective, the interaction between noscapine anticancer drug and human serum albumin (HSA) was investigated systematically under physiological conditions by using spectroscopic (absorption spectroscopy, fluorescence spectroscopy, Time resolve fluorescence, CD spectroscopy), electrochemistry (cyclic voltammetry) and computational method (molecular docking and molecular dynamic simulation). The Stern–Volmer quenching equation has been successfully applied and calculate Stern–Volmer quenching constant at different temperatures. The results show that noscapine quenched the intrinsic fluorescence of HSA through static quenching mechanism. The corresponding thermodynamic parameters ΔH , ΔG and ΔS were also calculated. The binding of noscapine and HSA resulted in the formation of noscapine–HSA complex and hydrophobic and hydrogen bond interactions played a major role in the complex stabilization. The distance r between the donor (HSA) and the acceptor (Noscapine) was obtained through fluorescence resonance energy transfer (FRET). Molecular docking indicated that the binding site of noscapine to HSA was located at site I. The results of synchronous fluorescence spectra, CD spectra and MD simulation indicated that the microenvironment and the conformation of HSA were changed noticeably due to the presence of noscapine. The results were further confirmed through cyclic voltammetry approach.

Key words: Noscapine, human serum albumin, hydrophobic interaction, docking.

Cost effective and energy saving gas sensing devices based on reduced graphene oxide

Ramesh Kumar and Amarjeet Kaur*

Department of Physics and Astrophysics, University of Delhi, Delhi 110007, India

**Email: amarkaur@physics.du.ac.in*

Many materials have been widely studied for gas sensing applications due to their own specific characteristics. The gas sensing devices based on metal oxide sensors have been thoroughly investigated due to their good sensing capability. However, these sensors hold an obvious disadvantage of requiring higher temperatures for their optimum operation. Also, the operation at elevated temperatures requires high power consumption and complex circuitry. The necessity of energy saving, room temperature operated gas sensors motivated researchers to look for alternate materials like conducting polymers. They exhibit rapid response and fast recovery, unlike most of conventional metal oxides sensors. However, these devices also have a serious issue with their environmental stability and get easily degraded. The focus of the researchers is now towards nanostructured gas sensing systems based on reduced graphene oxides, due to their high specific surface area as well as unique electrical properties such as high mobility and high signal to noise ratio.

In this report, the gas sensing performance of reduced graphene oxide based sensors is discussed. The reduced graphene oxide sensors are fabricated by the reduction of graphene oxide. The graphene oxide is reduced by chemical reduction as well as thermal reduction method. The reduction of the sample is explained on the basis of Raman spectra. The reduction of graphene oxide samples has been estimated on the basis of Tuinstra and Koenig relation. FT-IR studies indicate characteristic peaks at $1500\text{-}1600\text{ cm}^{-1}$ due to disordering in the samples during reduction. Furthermore, it shows the induction of defects in the graphene sheets. Reduction has enhanced electrical conductivity of reduced graphene oxide samples. The sample reduced with chemical method has shown promising potential for room temperature chemiresistive SO_2 gas sensor at ppm levels as low as 5ppm with reasonable sensitivity, selectivity and stability. It is also observed that the gas sensing property of reduced graphene oxide also depends upon reduction process.

Keywords: reduced graphene oxide, gas sensors, sensing mechanism

High contrast poly(aniline-co-anisidine) with higher stability and improved Electrochromic properties

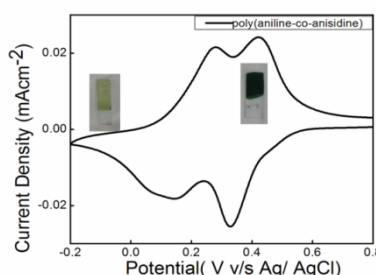
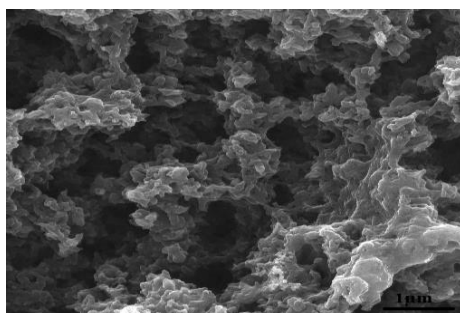
Jamdegni, Monika and Kaur, Amarjeet *

Department of physics and Astrophysics, Delhi University, Delhi-110007, India

*Email: amarkaur@physics.du.ac.in

The major harmful consequence of global warming can be seen as a continuously increasing temperature, which in turn increases the energy expenditure for air conditioning in buildings and vehicles. Such energy expenditure in this era where we are craving for energy is required to be treated in a different manner. Thus change in energy technology is the need of the hour. In this regard low power energy saving devices like smart windows are like boon. Smart window uses electrochromic material capable of altering its level of transmission by mere application of very low voltage say less than $1V$ ¹. Thus, such technology needs to be taken upto practical level of application and a lot of organic and inorganic materials have been taken for Electrochromic application, one of the such well characterized material is polyaniline. Its ample coloration, ease of synthesis, fast response make it an perfect material for Electrochromic application² but its low electrochemical stability has always remained an issue for practical application. Here we have taken two types of monomer units - an ortho substituted monomer unit i.e. anisidine along with the parent monomer aniline and then carried out polymerization with the idea that anisidine having strong electron donor group at its ortho position bulky this side substitution protect the charge carriers and impart stability.

Nanocomposite have been successfully synthesised by potentiostatic method in 3-electrode electrochemical cell. Composite structure has been confirmed by FTIR spectroscopy. FESEM investigation indicates morphology to be of 3-D porous network. Electrochemical and electrochromic investigation have been carried out using cyclic voltammetry, chrono-amperometry and UV-Vis spectroscopy. The synthesized composite switches its color from dark green (colored) to pale yellow(transparent) with the alteration of potential. The synthesized Composite has been found to exhibit better Electrochromic performance with 62% contrast at 568nm and is highly stable even after 5000 cycles which is far better compared with both of its individual component polyaniline and polyanisidine. Thus poly (aniline-co-anisidine) seems to be potential material for Electrochromic application.



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Performance of NiO-rGO based electrodes with proton conducting PVA based gel electrolyte for supercapacitor applications

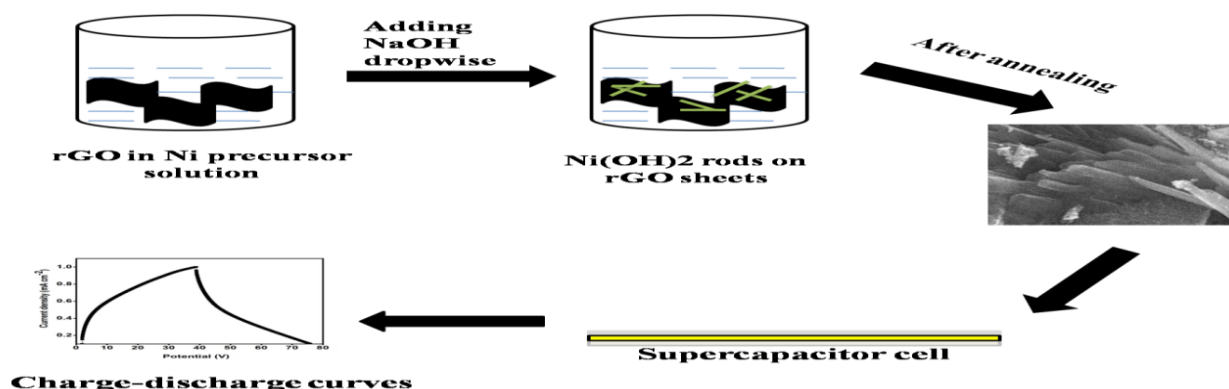
Deepika Jain, S.A Hashmi and Amarjeet Kaur*

Department of Physics and Astrophysics, Delhi University, Delhi, India

Email: - amarkaur@physics.du.ac.in

We have synthesized the composite of Nickel oxide-reduced graphene oxide (NiO-rGO) as electrode material along with the PVA-H₂SO₄ based gel polymer electrolyte for supercapacitor applications. The composite was synthesized via hydrothermal method in the presence of reduced graphene oxide. The morphology of the composite was analyzed by scanning electron microscopy (SEM) and the synthesis of the composite was confirmed by X-ray diffraction (XRD) technique. The supercapacitive performance of the composite was evaluated by testing the composite electrodes with PVA-H₂SO₄ based gel electrolyte using cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS). The composite demonstrates the maximum specific capacitance value of 3.8 F g⁻¹ which corresponds to energy density of 0.39 Whkg⁻¹ along with the power density of 840 Wkg⁻¹. The composite delivers stable performance for 4000 charge-discharge cycles. The EIS studies depict the high rate performance of composite electrode as indicated by the high Knee frequency (~ 380.9 Hz) and high pulse power. These attributes make it a promising electrode material for supercapacitors with long cycling stability.

Keywords: - Galvanostatic charge discharge, electrochemical impedance spectroscopy, reduced graphene oxide, cyclic voltammetry, polyvinyl alcohol.



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Dynamic and Nano Mechanical Properties of Graphene Oxide- Carbon Nanotube Hybrid Acrylonitrile Butadiene Styrene Composites

Jeevan Jyoti^{1,2}, Bhanu Pratap Singh^{1,2*}, S.R. Dhakate¹

¹*Advanced Carbon Products, Advanced Materials and Devices, CSIR-National Physical Laboratory, New Delhi -110012, India*

²*AcSIR-National Physical Laboratory, New Delhi-110012, India*

Corresponding author: Tel.: +91-11-45608460; Fax: +91-11-45609310

Email: [*bps@nplindia.org](mailto:bps@nplindia.org), bpsingh2k4@yahoo.com (B.P. Singh)

Acrylonitrile-butadiene-styrene (ABS) reinforced with MWCNTs, FCNTs and GCNTs hybrid Bucky paper (BP) were prepared via vacuum filtration and then hot compression. The Nano-mechanical and dynamic mechanical properties of these polymer composites were studied. The nanoindentation hardness and elastic modulus of GCNTs-ABS hybrid composites was 398.9 MPa and 7497.6 MPa, respectively as compared to pure ABS 248.5 MPa (Hardness) and 4500.7 MPa (elastic modulus) respectively, which have much higher than the MWCNTs-ABS and FCNTs-ABS composites. Other nanomechanical parameters such as plastic index parameter, elastic recovery, ratio of residual displacement after load removal and displacement at maximum load have also investigated. The improvement in the nanomechanical properties has also correlated with spectroscopic (Raman spectroscopy) and microstructural characterizations (scanning electron microscopy). The intensity ratio of "D" and "G" peaks have the strongly dependence upon the laser excitation energy. The amount of disorder in a nano-crystallite was given by the amount of border (one-dimensional defect) with respect to the total crystallite area, and this is a measure of the nano-crystallite size L_a . The distance between defects, L_D , have measured of the amount of disorder and also measure the defect density n_D . Largest the defect density and shortest the distance between the GCNTs filler made the strongest bonding between the ABS as compared to the other. The dynamic mechanical studied reveal efficient reinforced filler strongly depend upon dimension of filler and interaction between the filler and matrix. The dynamic mechanical properties of polymers strongly depend on the adhesion of filler, entanglement and cross link density of polymer chains with filler. GCNTs-ABS hybrid was more stiffness due to their perfect bending. These improvements were originated from the synergistic effect between GO and MWCNTs.

Keywords: Bucky paper, ABS, composites, Multiwalled carbon nanotube (MWCNTs), Functionalized carbon nanotube (FCNTs), graphene-oxide carbon nanotube (GCNTs), dynamic mechanical analyzer (DMA), nanomechanical and Raman analysis.

Energy harvesting from different materials using mechanical motion

Azad Puneet

Department of Electronics & Communication Engineering, Maharaja Surajmal
Institute of Technology, C-4, Janak Puri, New Delhi, Delhi 110058, India

Rubbing of two materials causes static electricity, which is the collection of electrically charged particles on the surface of a material. Some materials have a tendency of either giving up electrons or becoming positive (+) in charge or attracting electrons and becoming negative (–) in charge. This type of contact electrification is known as Triboelectric effect. This effect has been recently applied in energy harvesting to design and fabricate triboelectric nano-generators (TENGs) ¹. It is one of the most inexpensive and efficient mode of generation of electricity. Mechanical motion in daily life such as human walking ², rotation of tyres of vehicles ³, rotation of fan and motors can be converted to a source of generation of electricity. The basic phenomenon to generate a voltage depends on the type of material used. The simplest design is the rubbing or frequent contact of two materials, which has the tendency of attracting opposite charges as shown in Figure 1. The two materials having different electron affinity are brought in contact either vertically or in sliding fashion and opposite charges are produced on the materials. These charges are transferred to the two electrodes, thus used to generate a potential across them.

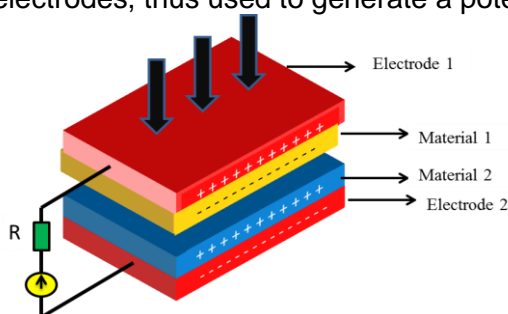


Figure 1: Operating principle of TENG

Different materials such as Aluminium and Copper, which have the tendency of attracting positive charges while materials such as Polytetrafluoroethylene (PTFE), Fluorinated ethylene propylene (FEP) and Polyimide film (like Kapton), which attracts negative charges are used for the generation of charges. Further, the charge is transferred in the two electrodes to generate a potential. While conducting experiments, it is observed that a combination of Aluminium-PTFE-Cu produces a potential of 5.4 volt on pressing of Al on the PTFE film. Similarly the combination of Al-FEP-Cu produces a voltage of 4.3 volt while Al-Kapton-FEP-Cu produces 3.9 volt. Rubbing of such combination of materials using a mechanical motion will produce tremendous amount of potential. This voltage is in the form of a.c. and is converted into d.c. using a rectifier circuit and can be used to operate electronic circuits or low power devices such as calculator, heart rate monitor, clock etc. In an experiment, the charging of various capacitors is observed by rubbing Al and FEP and the voltage reaches to a maximum of 17.196 volt ($1\mu F$) and 1.37 volts ($1000\mu F$) in 400 seconds. A battery of 2.4 volt is also charged and can be used to operate a device. Such studies are beneficial to understand the future perspectives of energy harvesting and its applications using different materials.

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A new approach for energy harvesting via strain mediated magnetic induced luminescence from Flexible composite laminates

Satbir Singh^{a,b,*}

^a*Alternative Energy Materials Section, Advanced Materials and Devices Division, CSIR- National Physical Laboratory, Dr K S Krishnan Road, New Delhi, 110012,*

^b*Academy of Scientific and Innovative Research (AcSIR), CSIR-National Physical Laboratory Campus, Dr K S Krishnan Road, New Delhi 110012, India*

^{*}*Email: satbirsinghbamrah@gmail.com*

Novel materials directly converting magnetic field into visible light are highly desirable for futuristic magnetic sensors for real-time visualization, remote sensing without making electric contact, nondestructive and noninvasive detection, for which magnetic sensors based on conversion of magnetic field input into electrical signals can't be used. Herein, we report a composite laminate system exhibiting strain mediated magnetic induced luminescence for efficient energy harvesting applications. The composite laminate system is designed by combining two separate polymer matrices of ZnS:Cu²⁺ and Fe-Co-Ni alloy in PDMS. The synthesized ZnS:Cu²⁺ phosphor, Fe-Co-Ni alloy and fabricated flexible composite layer were characterized to explore the structural/microstructural, morphological, photoluminescence and magnetic properties. Thus, our new approach for flexible composite laminate offers a paradigm shift to harvest energy by coupling of magnetic field, piezoelectric and photo-excitation effects.

Development of New Methanofullerenes And Their Transport Studies for Organic Photovoltaic Applications

Samya Naqvi and Rachana Kumar

CSIR-National Physical Laboratory

Advanced Materials and Devices Division (Flexible Organic Electronic Devices Group)

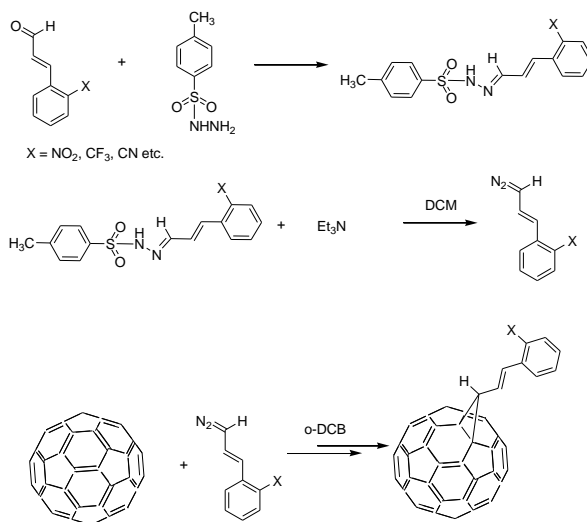
Dr. K. S. Krishnan Marg, New Delhi-110012

Email: samyanagviamu@gmail.com

The design of new organic functional materials, able to harvest maximum solar energy to accomplish the cheaper source of energy demands, is drawing the considerable attention of researchers in the area of organic photovoltaics (OPV). This study involves the development of new fullerene derivatives bearing electron withdrawing units covalently attached exohedrally to fullerene [60] as well as their charge carrier transport properties. The presence of electron withdrawing units as constituents of the fullerene framework increases the electron accepting properties in fullerenes. For functionalization of fullerenes commonly used strategies are [2+1], [2+2], [3+2], and [4+2] cycloadditions, nucleophilic addition reactions and radical reactions.

Phenyl[C61]butyric acid methyl ester (PC61BM) and [6,6] Phenyl[C71]butyric acid methyl ester (PC71BM) are the most well known acceptor materials used in organic photovoltaics in combination with almost all donor materials. To achieve highly efficient solar cells, we focused on the synthesis of stable fullerene[60] based acceptor molecules. These acceptor molecules showed broader and stronger absorption in the visible region of the solar spectrum. The most straight forward method to improve the performance of solar cell is through its open circuit voltage, the higher open-circuit voltages are reasonably attributed to the higher LUMO levels of the fullerene derivatives. The modified C₆₀ was expected to improve the morphology of active donor/acceptor blend layer in order to increase the carrier collection efficiency.

Charge carrier transport property is an important parameter for solar cell characterization. The cells are fabricated in such a way that the carriers of opposite sign have been selectively blocked by choosing the relevant contacts of different work function.



In this study we will focus on the synthesis of different fullerene derivative via cyclopropanation reactions i.e., amine assisted 1,3 dipolar cycloaddition (AACA) reactions. This is the first reported method for the synthesis of fullerene derivatives from diazo compounds. Also the electron transport in new methanofullerenes was

investigated and the electron current in our products is space charge limited through which the electron mobility has been calculated by J-V measurements.

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Development of Fullerene based Single Ambivalent Materials for Organic Photovoltaic Applications

Neha Gupta and Rachana Kumar
CSIR-National Physical Laboratory

Advanced Materials and Devices Division (Flexible Organic Electronic Devices Group)

Dr. K.S. Krishnan Marg, New Delhi-110012

Email: nehagupta6342@gmail.com

Organic photovoltaics (OPV) is one of the most reliable and long-term solution for the clean and renewable energy and possess several advantages like lower manufacturing cost, flexible and lightweight solar cells, semi transparent and fabrication can be done by roll-to roll process. In bulk heterojunction (BHJ) solar cells, conjugated polymers donors and fullerene based acceptors have frequently been used to form a interpenetrating phase-separated network composite which allows free charge carrier generation, charge transport and collection for generation of photocurrent. The nano-morphology has a great impact on the efficiency of organic solar cells and to achieve higher power conversion efficiency, a large effort has to be paid on the fabrication conditions. Besides, the optimized morphology of the active layer which is not so stable due to the evolution of fullerene aggregation with time, resulting in interfacial reduction and simultaneously deteriorates the device performance. To deal with these stability issues in bulk heterojunction cells, there comes a new idea of development of a single ambivalent material containing donor and acceptor (DYAD) parts which has the capability of ensuring the process of light absorption, exciton formation, exciton dissociation, charge transport and collection. The strategy lies behind the synthesis of DYAD material is to link the donor and acceptor molecules covalently with spacer linker.

Here in our present work we are focussing on the synthesis of fullerene based acceptor molecules like Phenyl[C61]butyric acid methyl ester (PC61BM), Phenyl[C61]butyric acid pentyl ester (PC61BP) and [6,6] Phenyl[C71]butyric acid pentyl ester (PC71BP) via cyclopropanation reactions using our cost-effective and eco-friendly methodology, i.e., amine assisted 1,3 dipolar cycloaddition (AACA) reactions. On the other hand for the donor molecules we are synthesizing porphyrin based donor molecules which are meso substituted and that can be covalently linked with the fullerene based molecules. All the synthesized materials were characterized by using various characterization techniques like NMR, MALDI-TOFF, FTIR, UV-vis and charge transfer studies have been performed by ultrafast transient absorption spectroscopy. These materials have been tested in organic solar cells as single material in active layer.

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INDIGENOUS SYNTHESIS OF POLYMER BASED ORGANIC THERMOELECTRICS

Jyoti Garg , Rachana Kumar and Ajay Dhar

CSIR- National Physical Laboratory

Advanced Materials and Devices division (Flexible Organic Electronic Devices Group)

Dr K. S. Krishnan Marg, New Delhi- 110012

Email: zyotigarg03@gmail.com , rachanak@nplindia.org

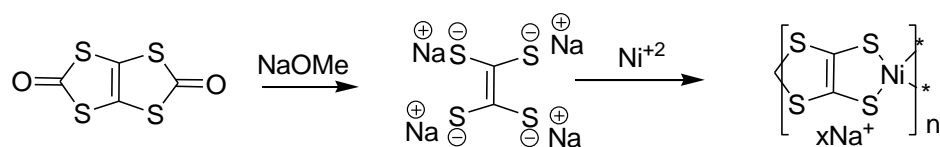
As this planet is struggling with harmful effects of greenhouse gases, scientists around the world is searching for alternative energy other than fossil fuels. Thermoelectricity is one such area which need to be explored through which huge amount of unusable heat or waste heat can be converted to electricity. The efficiency of a thermoelectric material system is defined by a dimensionless parameter thermoelectric figure of merit, $ZT = S^2 \sigma T / \kappa$, where S , σ , κ and T are the Seebeck coefficient (also termed as thermopower), electrical conductivity, thermal conductivity and absolute temperature, respectively. Though inorganic thermoelectric has been studied extensively due to their high σ , but less attention is paid to organic thermoelectric.

It has been demonstrated that p-type organic material poly (3,4-ethylenedioxythiophene) exhibits a high ZT value of 0.25. This finding is exciting and encouraging, for the first time it shows that organic materials could also be very good thermoelectric materials despite their intrinsic low conductivity.

Yimeng Sun et.al found that n-type materials poly [$\text{Na}_x(\text{Ni-ett})$] and poly [$\text{K}_x(\text{Ni-ett})$] exhibit excellent TE characteristics. They found that n-type materials poly [$\text{Na}_x(\text{Ni-ett})$] and poly [$\text{K}_x(\text{Ni-ett})$] exhibit high ZT values of 0.1 to 0.2 around 400 K (which are among highest for organic materials). We have synthesized the polymer poly [$\text{Na}_x(\text{Ni-ett})$] indigenously as per the given scheme, we have used a surfactant while synthesizing it, which made it more soluble.

The structure was characterized by FT-IR and UV-Vis spectroscopy. The thermoelectric properties like Seebeck coefficient, Power factor was determined to be $5.6 \mu\text{V/K}$ and $1.83 \times 10^{-5} \text{ Wm}^{-1}\text{K}^{-2}$.

Scheme:



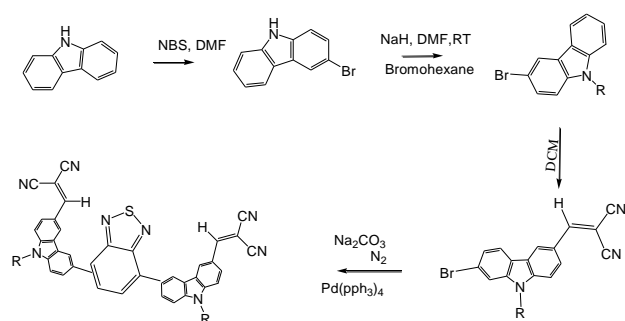
Synthesis, photophysical, and electrochemical studies on Carbazole based small molecules for heterojunction solar cell

Neelam Kumari and Rachana Kumar

Advanced Materials and Devices Division (Flexible Organic Electronic Devices Group), National Physical Laboratory, New Delhi

Email: neelamchem11@gmail.com

Due to the Optoelectronic properties of the non-fullerene based acceptors, the photovoltaic devices made up with P3HT, PTB7 as Donor materials shows promising result. Small molecule based organic solar cells are designed in push-pull structure in which coupling of Donor-Acceptor moieties give high device performance. Coupled electron-donor (D) and electron-acceptor (A) unit construct highly conjugated material which exhibit efficient charge transport, maximum light absorption, low band gap, strong intermolecular interaction and behaves like semiconductor. Donor – Acceptor approach such as, perelyene, carbazole, flourene , indole unit use as donor moieties as end groups and benzothiadiazole(BT) as electron deficient heterocycles have been mostly investigated for (BHJ) solar cells.



A new small molecule based on carbazole has been synthesized and characterized which is easily processable and cost-effective. The molecule may be shows high thermal stability which will be characterized by thermo-gravimetric analysis (TGA). Carbazole based small molecule has ability to form good thin film and is air stable as well. Its electrochemical and photo-physical studies ensure a compatible HOMO-LUMO energy levels which are potentially useful as an efficient electron acceptor material in bulk-heterojunction solar cell combined with electron donor materials such as poly-3-hexylthiophene (P3HT) or copper(II)phthalocyanine. Significant photoluminescence quenching of donor:acceptor (small molecule) blends will be observe. The structure of the acceptor molecule has been established by different spectroscopic methods like FTIR, UV-vis, NMR, MALDI-TOFF, PL, CV and charge transfer studies have been performed.

Keywords: Carbazole, Malononitrile, Bulk-heterojunction solar cell, HOMO-LUMO energy levels.

Dielectric and/or semiconducting nanolayers by atomic layer deposition for surface passivation of crystalline silicon

Panigrahi, Jagannath, Panwar, Vandana, Singh, Rajbir and Singh Parakram
*Academy of Scientific and Innovative Research (AcSIR), CSIR-National Physical
Laboratory Campus, New Delhi-110012 (India)*
*Inorganic Photovoltaic Devices Group, CSIR-National Physical Laboratory, Network
of Institute for Solar Energy, New Delhi-110012 (India)*

Dielectric or semiconducting nanolayers are emerging as key components in today's highly efficiency silicon solar cells such as PERC. The most successful materials are SiO_2 , $\text{SiN}_x\text{:H}$ and Al_2O_3 due to their excellent material properties for surface passivation and light trapping/management. These passivation layers provide high level of chemical passivation by effectively reducing the density of silicon surface states, which act as recombination centers for excess photo-generated charge carriers. Additionally, these materials provide strong field-effect passivation because of high density of intrinsic fixed charges. However, novel solar cell concepts demand for dielectric nanomaterials with additional functionalities such as simultaneous applicability as a passivation, antireflection and carrier selective transport layer. These require the tailoring of charge states in these layers by suitable combination of dielectrics or semiconducting layers. Recent developments show that these functionalities can be realized in multi-oxide nanolaminates including Al_2O_3 , HfO_2 and ZnO sublayers.

This study deals with the silicon surface passivation by ALD deposited bilayers and multilayers of oxides such as $\text{HfO}_x/\text{AlO}_x$ and $(\text{ZnO}/\text{AlO}_x)$. A significant improvement in the effective minority carrier lifetime of n-Si ($\sim 1.3\text{ms}$) is observed after deposition of a few nanometers of HfO_x layers (3-7nm) over few nanometers of AlO_x (7-3nm) compared to the single layers of AlO_x ($\sim 0.6\text{ms}$) and HfO_x ($\sim 0.8\text{ms}$) layers of $\sim 10\text{nm}$ thick. This enhancement in the surface passivation is found to be due to a significant enhancement in the effective charge density in the bilayer system. Similarly, high effective minority carrier lifetime of 1.6ms is obtained with multilayers of ZnO/AlO_x deposited on Si by ALD as compared to single layer of ZnO ($30\mu\text{s}$). In addition, suitability of ZnO and AZO layers as quarter-wave antireflection coating on Si are also studied.

Atomic layer deposition of aluminium oxide and hafnium oxide films for silicon surface passivation and their application in solar cell.

Singh, Rajbir, Vandana, Panigrahi, Jagannath and Singh, Parakram
*Academy of Scientific & Innovative Research (AcSIR), CSIR-National Physical
Laboratory
(CSIR-NPL) Campus, New Delhi
Inorganic Photovoltaic Devices Group (Network of Institutes for Solar Energy) CSIR-
NPL, New Delhi, India*

Interface engineering is of vital interest for solar cell manufacturing as the properties of interfaces between different materials play a decisive role in the performance of photovoltaic (PV) devices. So dielectric thin-film deposited on top of solar cells serve important roles as a surface passivation layer to reduce the surface recombination loss and as well as an anti-reflection layer for photon management for crystalline silicon (c-Si) solar cells. As the thickness of c-Si solar cells decreases in order to lower down the manufacturing cost of solar cells, Si surface passivation becomes a more and more important issue for high efficiency solar cells. Therefore, a variety of dielectric materials have been proposed for the surface passivation of solar cells, such as silicon dioxide (SiO_2), amorphous silicon nitride ($\text{a-Si}_3\text{N}_4$), amorphous silicon (a-Si), aluminium oxide (Al_2O_3) and hafnium oxide (HfO_2). Beside the use of dielectric thin films, Si surface passivation also depends on the deposition techniques, surface cleaning, and types of Si substrates. Among different deposition techniques, atomic layer deposition (ALD) provides a unique feature for the growth of thin films with excellent conformity and thickness control down to atomic levels which is suitable for complex surface textured surface and large-size industrial solar cell. The application of ALD in energy research has received increasing attention in recent years.

In this work, the versatility of ALD deposited oxides in c-Si solar cells will be discussed. Atomic-layer-deposited aluminium oxide (AlO_x) and hafnium oxide (HfO_x) are used as passivation layer on silicon surface. AlO_x and HfO_x provide surface recombination velocity (SRV) of $\sim 6\text{cm/s}$ and 40cm/s respectively. Atomic-layer-deposited aluminium oxide films are applied as rear-surface-passivating dielectric layer to passivate rear of industrial silicon solar cells. The surface passivation of low-resistivity p-type silicon by the negative-charge-dielectric AlO_x is confirmed on the device level by an energy conversion efficiency of nearly 17% which is absolutely 1% higher than the control cell. These results are obtained for a 30 nm AlO_x film deposited using thermal ALD process and covered by a 60-80 nm plasma-enhanced-chemical-vapour-deposited silicon nitride (SiN_x) layer, resulting in a low rear surface recombination velocity (SRV).

Polyaniline-Silver core-shell nanocomposite as an energy efficient rapid hydrazine chemiresistors

Vishal Chaudhary and Amarjeet Kaur
amarkaur@physics.du.ac.in

*Department of Physics and Astrophysics
University of Delhi, Delhi-110007, India.*

An advanced core-shell type nanocomposite (PAg) of polyaniline (PAN) and silver has been synthesized with the assistance of methyl-orange. The core-shell type structure of synthesized nanocomposite has been confirmed by using high resolution tunnelling electron microscopy (HRTEM) and surface enhanced Fourier transform infrared spectroscopy (SE-FTIR). The chemiresistors were fabricated by using cost-effective spin coating technique. The sensing response of PAg chemiresistor was found to be two-fold enhanced as compared to that of PAN based chemiresistor. Furthermore, the fabricated chemiresistor possess rapid response towards hydrazine with good recovery. The fabricated chemiresistor works at room temperature, thus simplifying the electronic circuitry by exclusion of micro heating assemblage and reducing the requirement of energy for operation. The mechanism of sensing is explained in terms of charge transfer between p-type polyaniline and reducing hydrazine, where silver plays role of a catalyst by increasing the pace of interaction. This study opens a new window for commercial development of energy efficient sensors to detect low parts per million concentration of hydrazine at room temperature.

Keywords:

Core-shell hybrid, chemiresistor, SE-FTIR, energy efficient.

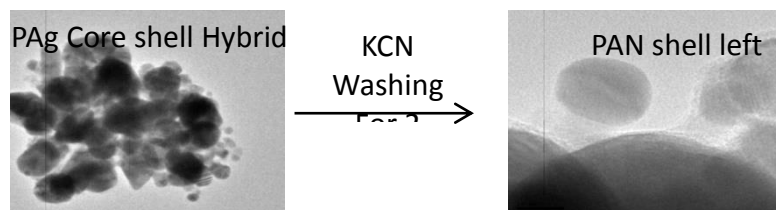


Fig.1: Conformation of PAg core-shell structure by KCN washing method.

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Wet chemically etched silicon nanowire arrays based black solar cells

Sanjay K. Srivastava*, Prashant Singh, C.M.S. Rauthan, P.K. Singh
*Inorganic Photovoltaic Devices Group, Advanced Materials & Devices Division,
CSIR-National Physical Laboratory, New Delhi-110012, India.*
**E-mail: srivassk@nplindia.org; sksrivastava78@gmail.com*

Semiconductor nanostructures are promising building blocks for next generation photovoltaic (PV) devices with improved energy conversion efficiencies and lower cost. Silicon based nano-structured solar cells offer several advantages, including the natural silicon abundance, lack of toxicity, and compatibility with mature micro-electronics fabrication techniques. Vertically-aligned silicon nanowires (SiNWs) array exhibit low reflection and strong broadband absorption and may be used as antireflection surface or as the active layer in solar cells. In particular, SiNWs array incorporating radial p-n junctions provide advantageous optoelectronic properties that may relax high quality material requirement, enabling lower-cost PV cells.

Herein we present a systematic study on wet chemically etched SiNWs array based p-n junction solar cells. Large area arrays of vertically aligned SiNWs of tunable length and diameters ~100-300 nm have been fabricated at room temperature by a single step Ag catalyzed wet etching of B-doped silicon (100) wafers. The reflectance properties of the array surface were investigated to utilize them as a cost effective anti-reflection coatings in silicon solar cells. Reflectivity as low as 2 % in 300-700 nm with an average R_{λ} of < 4 % in the spectral range (300-1100 nm) of interest for silicon solar cells has been shown. The SiNWs array based “black” solar cells employing the low reflective property of the nanowires array have been fabricated wherein the metal contact quality as good as on planar silicon solar cells has been achieved. The SiNWs array solar cells have n^+pp^+ structure. The emitter (n^+) is made by conventional phosphorus diffusion and thermally evaporated Al used to create a back surface field (p^+) layer. Front and rear electrodes are made using Ti/Ag deposition through metal mask followed by annealing in forming gas. Electrical properties of the SiNWs based cells such as I-V, quantum efficiency, LBIC, diffusion length and reflectance measurements are investigated to calculate cell parameters and are compared with that of planar cells (without SiNWs). Significant enhancement in short circuit current density (>25%) and efficiency (an absolute ~1 %) have been achieved in the SiNWs solar cells as compared to the planar reference cells. Detailed structural characterization of the SiNWs (both pre- and post p-n junction formation) is carried out using high resolution scanning and transmission electron microscopes and energy dispersive X-ray analysis to understand the device structure. The preliminary results indicate the formation of radial p-n junction in the nanowires. However, further investigations are needed; particularly using an *in-situ* nano-probing/analytical tool for the confirmation of radial junction in the nanowires.

Investigation on tunneling behavior superconductor-ferroelectric-ferromagnetic hetero-structure thin films for energy harvesters

Ravikant^{1,2} Ashok Kumar^{1,2,*} V. N. Ojha¹,

¹*CSIR-National Physical Laboratory, Dr. K. S. Krishnan Marg, New Delhi 110012,*

²*Academy of Scientific and Innovative Research (AcSIR), CSIR-National Physical Laboratory (CSIR-NPL) Campus, Dr. K. S. Krishnan Road, New Delhi 110012, India*

Email: ashok553@nplindia.org

Quantum disturbances can leak through a high potential barrier height when their critical thickness is less than 10 nm, necessary for tunneling effects. To investigate the quantum tunneling effects, we investigate epitaxial LAO/BSCCO(100 nm)/PZT(5 nm)/LSMO(50 nm) for tunneling effect and MgO/LSMO(50 nm)/BSCCO(5 nm)/PZT(5 nm) for magneto-caloric and piezo-force microscopy (PFM) effects. These films were grown by pulsed laser deposition system under different growth conditions. X-Ray Diffraction patterns of these hetero-structures suggest the formation of each individual layers along the direction of substrate plane. Surface geography and PFM data illustrate the polar nature of PZT even for the dimension of 5 nm which is one of the essential conditions. Current-voltage characteristic of bulk superconductor Bi-Sr-Ca-Cu₂-O_x (in dimension 5mm x 5mm) carried out using four probe method show that superconducting phase transition occur at 88.84 K, same target was used for thin films fabrication. Tunneling effects for these hetero-structures were carried out at room temperature and at 77 K; a signature of multi-states resistance was observed at low temperature. A robust magneto-caloric effect was obtained for these nanostructures suggest a potential candidate for solid-state renewable energy efficient refrigerator.

Keywords: Tunneling, Ferroelectric, Quantum Disturbance.

Near UV Photodetector and Photo-driven Polarization Switching in Ferroelectric Thin films

Hitesh Borkar, Ashok Kumar *

CSIR-National Physical laboratory, New Delhi, India 110012

**Corresponding Author: ashok553@nplindia.org*

Photosensitive ferroelectric materials exhibit various photoferroelectric phenomena due to the strong influence of nonequilibrium charge carriers on polarization. These phenomena are essential for a number of applications including photo driven actuators and sensitive photo detectors. In this work, the effect of illumination on ferroelectric, dielectric and current-voltage properties is investigated in Bi and Li doped lead zirconate titanate ($\text{Pb}_{0.6}\text{Li}_{0.2}\text{Bi}_{0.2}\text{Zr}_{0.2}\text{Ti}_{0.8}\text{O}_3$ -PLBZT) thin films, which show promising candidates for multi functional applications. We synthesized PLBZT/LNO (thickness~250 nm) thin films on LAO substrate by pulsed laser deposition technique. Ferroelectric switching were observed at 10 V under different illuminated conditions, corresponding derived displacement current also shows the same type of switching. Photo driven polarization switching and its reproducibility were checked at different intervals of short and long period of time. Dielectric constant and loss were measured over wide range of frequency from 100 Hz to 1 MHz under dark and light condition, which indicate enhancement in dielectric constant and decreases in tangent loss under illuminated condition. In-plane photo detection was measured on semi transparent gold electrode under different conditions i.e. dark, under illumination of white light source, and laser having wavelength 405 nm. Lifetime, action of absorbing and continuing switching in current is measured by fatigue and retention. A direct effect of the photo driven ferroelectric polarization and current-voltage is observed under essentially nondestructive conditions. These results may be useful in the development of new energy saver devices, such as photo-ferroelectrics nonvolatile memory, opto-electronics, photo-voltaic and photo-detectors, etc.

Unipolar resistive switching behaviour of SrTiO₃ and FeSrTiO₃ thin films for non-volatile memory applications

Atul Thakre^{1,2}, Ashok Kumar²

¹*Academy of Scientific and Innovative Research (AcSIR), CSIR-National Physical Laboratory Campus, Dr. K. S. Krishnan Marg, New Delhi 110012, India*

²*CSIR-National Physical Laboratory, Dr. K. S. Krishnan Marg, New Delhi 110012*

Email: ashok553@nplindia.org

A repeatable unipolar resistive switching (URS) was successfully observed in sol-gel derived perovskite type Strontium Titanate (STO) and Fe doped Strontium Titanate (FeSTO) thin films, deposited on FTO glass substrate by spin-coating technique. The surface topography of the films was characterized with atomic force microscopy. In order to thoroughly explore the conducting mechanism in RS phenomena, current-voltage measurements and Impedance parameters behaviour with frequency were analyzed for both resistive states (High resistance state (HRS) and Low resistance state (LRS)). The devices Au/STO/FTO and Au/FeSTO/FTO offer a resistance ratio of HRS and LRS ($R_{\text{off}}/R_{\text{on}}$) around 10^3 to 10^4 , long stable retention characteristics for 10^4 s and a distinguished non- overlapping voltage window of $\sim 2\text{V}$ for SET and RESET operations.

**Development of Rare Earth-Free Permanent Magnetic
Material for Energy Applications - ZrCoFeB Alloy**

Christopher Nithya, Anand Kritika, Singh Nidhi, Gupta Anurag and Dhar Ajay
*Council for Scientific and Industrial Research - National Physical Laboratory,
Dr. K.S. Krishnan Road, New Delhi-110012, India*

The escalating costs of rare-earth elements have triggered the development of rare earth free permanent magnetic materials^{1,2,3} which have vast applications, especially in energy generation and conservation sectors. In the current study, the magnetic properties of rare-earth free alloy $\text{Zr}_2\text{Co}_{9.5}\text{Fe}_{1.5}\text{B}$ have been investigated. These alloys were synthesized by repeated arc-melting to produce the master alloy, which was subsequently melt-spun in form of continuous nanocrystalline ribbons at a wheel speed of 20m/s. The X-ray diffraction patterns of these alloys, confirmed a presence of magnetic hard phase Co_5Zr in the annealed melt spun ribbons. It was observed that the heat treatment of the melt-spun ribbons resulted in the increase in coercivity (H_c) and optimized doping of Fe was effective in improving the magnetic properties with high saturation magnetisation (M_s) values. Typically the melt spun alloy, $\text{Zr}_2\text{Co}_{9.5}\text{Fe}_{1.5}\text{B}$, annealed at optimized conditions, yielded an $M_s \sim 91.7$ emu/g, $M_r \sim 49$ emu/g and $H_c \sim 1.64$ kOe with $(BH)_{\max} \sim 2$ MGOe at room temperature. These melt-spun alloys were characterized for their structure employing field emission scanning microscopy which was correlated with their magnetic properties.

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Study of Resistive Switching Mechanism involving Drift and Diffusion of Oxygen Vacancies in Polycrystalline Nb₂O₅

Deswal, Sweety 1,2, Kumar, Ashok 1,2 and Kumar, Ajeet 1,2

1AcSIR-National Physical Laboratory, Dr. K.S. Krishnan Marg, New Delhi 110012

2Academy of Scientific and Innovative Research, CSIR-National Physical Laboratory campus, Dr. K. S. Krishnan Marg, New Delhi 110012

[Email: kumarajeet@mail.nplindia.org](mailto:kumarajeet@mail.nplindia.org)

Oxide based resistance switching is promising for applications in resistive random access memory (RRAM) devices due to their fast switching speed, low power consumption, high retention power and durability. Among various transition metal oxides, Niobium pentoxide (Nb₂O₅) is also a very promising material for resistive switching devices in both amorphous and crystalline phases. A very few reports are available with study of conduction parameters of Nb₂O₅ thin film based resistive switching devices. In the present work, we investigated unipolar resistive switching with switching mechanism of polycrystalline Nb₂O₅ thin film. The Pt/Nb₂O₅/Al device with orthorhombic crystalline phase prepared by reactive sputtering method and ex-situ annealing, showed non-volatile reproducible unipolar switching with ON/OFF resistance ratio of 10³ or higher. The large ON/OFF ratio of the device makes it a desirable material for future memory devices. The range of SET and RESET voltage was 1.0-2.0 V and 0.3-0.8 V, respectively, depending on devices and their dimension. The charge carriers followed ohmic and space charge limited conduction (SCLC) behaviour in low resistance state (LRS) and high resistance state (HRS) states, respectively. A model based on drift and diffusion of oxygen ion vacancy is presented to explain the conducting filament formation and impedance spectroscopy for current-filament dynamics.

Waste derived Li-S Battery Cathode Materials

Shukla, Swapnil,^a Ghosh, Arnab,^b Mitra, Sagar^{b,1} and Lochab, Bimlesh^{a,1}

^aDepartment of Chemistry, School of Natural Sciences, Shiv Nadar University,
Gautam Budh Nagar, Uttar Pradesh 203207, INDIA

^bElectrochemical Energy Storage Laboratory, Department of Energy Science and
Engineering, Indian Institute of Technology, Bombay, Powai, Mumbai 400076, INDIA.

¹E-mail: sagar.mitra@iitb.ac.in, bimlesh.lochab@snu.edu.in; sagarmitra@iitb.ac.in

In the view of increasing energy demands, secondary storage energy devices are receiving widespread attention. Amongst the various devices under exploration, Lithium Sulphur (Li-S) batteries are gathering immense interest owing to inherently high theoretical energy density (2600 Whk/g) and capacity (1672 mAh/g) of elemental sulphur (S) along with its abundant availability.^{1,2} However, certain drawbacks viz. sulfur dissolution in the electrolyte leading to poor cyclability and reduced performance have impeded the further development of these devices. Recent measures to counter these drawbacks pertain to inverse vulcanization strategy synthesising polymer composites with high loadings of sulphur with latter entrapped by means of chemical confinement.¹ In this study, sustainable benzoxazines have been explored as novel comonomers to yield polysulphur copolymers with high loadings of S. These copolymers were derived from a solventless melt based strategy utilising sustainable monomers such as sulphur (industrial waste) and cardanol based benzoxazine (agro waste).³ Also, these polymeric systems were found to effectively address several conventional shortcomings of Li-S batteries.⁴ To further enhance the performance of these copolymers as cathodic entities, conductive fillers were incorporated. The two conductive fillers utilised, include commercially obtained Multi Wall Carbon Nanotubes (MWCNT)⁵ and sustainably synthesised reduced graphene oxide.⁶ Both the fillers were incorporated in different weight percentages and resulting performance was compared to ascertain their efficacy and economic viability. Hence a sustainable alternative polymer composite was studied for its utility as a cathode in Li-S batteries.

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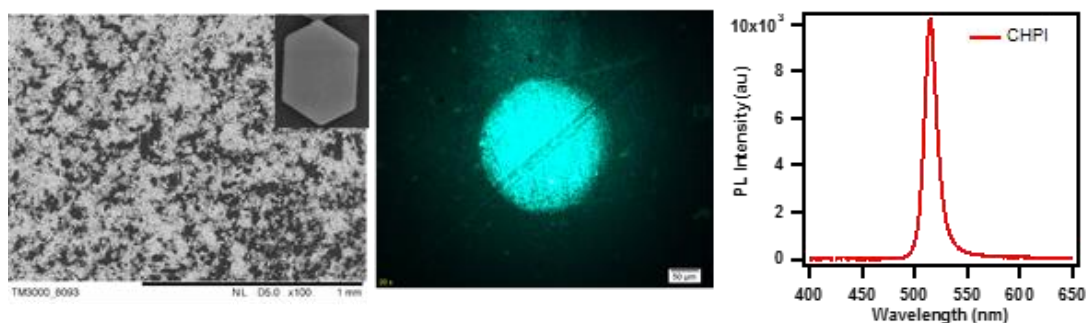
Single step fabrication of two-dimensional inorganic-organic perovskite luminescent crystals

Pawan K. Kanaujia, Indraj Singh and G. Vijaya Prakash

Nanophotonics Lab, Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi 110016, India.

Email: kanaujiapk09@gmail.com

Single step fabrication of two-dimensional (2D) inorganic-organic (IO) perovskite ($(R-NH_3)_2MX_4$, hexagonal nano/micro crystal has been carried by chemical route method. Where R is an organic moiety (C_nH_{2n+1} , $C_6H_5C_nH_{2n}$ etc.), M is a divalent metal (Pb^{2+} , Sn^{2+} etc.) and X is a halide (such as I^- , Br^- and Cl^-). Earlier we have also reported the fabrication of perovskite hexagon nanosheets by electrodeposition method in a two-step process. These 2D materials are stack of corner-sharing PbI_6 octahedra layers, separated by $R-NH_3$ cations via hydrogen bonding in the form of natural multiple quantum well (MQW) structures. A systematic study has been carried out to understand the growth reaction and optical properties of these crystals. These systems exhibits highly excitonic luminescent nature due to quantum and dielectric confinement effects at room-temperature. This low cost, easy fabrication technique for easy crystal growth can be a potential candidate for optoelectronic device applications.



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Tuning of optoelectronic properties for donor materials in organic solar cells: Thiophene based *block* polymers

Dinesh Bhardwaj^{1,2}, *Shahjad*^{1,2}, *Asit Patra*^{1,2,*}

¹Academy of Scientific and Innovative Research (AcSIR), CSIR-National Physical Laboratory Campus, ²Flexible Organic Energy Devices, Advanced Materials and Devices, CSIR-National Physical Laboratory, Dr. K. S. Krishnan Marg, New Delhi-110012, India

Thiophene-based conjugated polymers are among the most studied organic materials and are one of the most prominent commercially used materials in the conducting layers in photovoltaic cells. Block copolymers attracted a lot of interest in optoelectronic devices due to its tunable physical and chemical properties namely band gap, optical absorption, morphology, nanoscale phase separation, solubility and stability so forth. Block copolymers are consists of two or more covalently linked homopolymer blocks with distinct units. Generally, the block copolymers are significantly different in chemical and physical properties compared to their homopolymers. Polythiophene (PT) and poly(3,4-ethylenedioxythiophene) (PEDOT) and their derivatives are the most studied conjugated polymers, while PT having wide band gap (~ 2.05 eV) and PEDOT having narrow band gap (~ 1.65 eV). The block copolymers using these two units may generate novel properties for optoelectronic applications.

In the present work, poly(3-hexylthiophene)-*block*-poly(hexyl-3,4-ethylenedioxythiophene) (P3HT-*block*-PEDOT-C₆) copolymers were synthesized by Kumada catalyst transfer polymerization using different molar ratios of the components. Homopolymers, P3HT and PEDOT-C₆ were also obtained by using the conditions described for block polymers for comparison purpose. The block copolymers were characterized by using ¹H NMR spectroscopy. The optoelectronic and morphological properties of the resulting polymers were measured using UV-vis spectra, cyclic voltammetry and SEM images. The experiments results clearly indicated that the block copolymers show significant different properties compared to their constituent homopolymers, which are may be potential member for optoelectronic applications. Finally, we have successfully fabricated OPV device using indigenous development of P3HT in the device geometry of ITO/MoO₃/P3HT:PCBM/Al in ambient condition and found comparable results to commercial available P3HT.

Keywords: Homopolymer; *block*-copolymer; P3HT-*b*-PEDOT-C₆; optoelectronic properties.

Hole transport materials for excitonic solar cells: Poly(3,4-ethylenedioxythiophene) and its derivatives.

Sonal Gupta^{1,2}, Preeti Yadav^{1,2}, Ranoo Bhargav^{1,2}, Vikash Agarwal^{1,2}, Asit Patra^{1,2*}

¹Academy of Scientific and Innovative Research (AcSIR), CSIR-National Physical Laboratory Campus, ²Flexible Organic Energy Devices, Advanced Materials and Devices, CSIR-National Physical Laboratory, Dr. K. S. Krishnan Marg, New Delhi-110012, India

Hole transport materials (HTMs) in excitonic solar cells play an important role in device performance and stability for possible commercial applications. Several HTMs based on organic, inorganic and transition metals have been reported in literature. Water soluble poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) is the most successfully used HTM in excitonic solar cells, while presence of PSS, influences the device stability and degradation. Transition metal based oxides like MoO_x, VO_x, CuSCN so forth have been successfully reported as HTM as a replacement of PEDOT:PSS. Generally, hole transport layers (HTLs) are deposited by thermal deposition (small molecule and inorganic materials) and solution processable (organic materials and inorganic materials) for device fabrication.

Here, we report PSS free PEDOT and its derivatives as a novel solution processable HTM for excitonic solar cell. The PEDOT as a HTL was obtained by solid state polymerization of 2,5-dibromo-3,4-ethylenedioxythiophene on ITO coated glass by heating. Power conversion efficiency (PCE) was achieved up to 1.70% in device structure of ITO/Ssp-PEDOT/active layer/Al under ambient conditions. Furthermore, PSS free electropolymerized films of PEDOT and its derivatives were obtained as HTL to overcome the stability problem of devices. PCE of ~2.43% and stability of ~2000 hrs has been observed in device configuration of ITO/e-PEDOT/P3HT:PC₆₀BM/Ca/Al.

Keywords: Excitonic solar cells, Hole transport materials, PEDOT, Power conversion efficiency.

Sub-nano crystalline Silicon thin film for solar cells

Mansi Sharma^{1,2}, Deepika Chaudhary^{1,2}, S. Sudhakar¹, and Sushil Kumar^{1,2} **

¹*CSIR Network of Institutes for Solar Energy, CSIR – National Physical Laboratory,
Dr. K.S. Krishnan Marg, New Delhi-110012, India*

²*Academy of Scientific and Innovative Research (AcSIR), New Delhi-110012, India*

**Corresponding author. Tel: +91 11 45608650; Fax: +91 11 45609310;

E-mail: skumar@ nplindia.org

Hydrogenated amorphous/micro/nano-crystalline silicon (a-Si:H/ μ c-Si:H/nc-Si:H) thin film based solar cells have gained enormous attention in the scientific community owing to their preeminent opto-electrical properties with the benefit of cost effective device formation over large surface area. However, the respective devices offer certain limitations due to the meta-stability of a-Si:H under light illumination (~10 % to 30 % degradation during initial hours) and lower efficiencies of micro/nano-crystalline device as an effect of limited photo-response with the effective distribution of crystallites within amorphous phase (~ 10.7 %). Thus, there is a need to further explore the existing phase in a way to get efficient as well as stable solar cell structure.

Present work discusses the structural modifications in conventional a-Si:H material deposited using Plasma Enhanced Chemical Vapor Deposition (PECVD) technique which highlights the crystallite formation within the boundaries of micro to nano crystallite silicon thin films. These phases were generalized as sub-nano crystalline silicon phases. The observed crystalline volume fraction of these sub-nano crystallites found to vary from ~18 % to 30 %. The crystallite growth can probably be visualized starting from the partial nucleation to coalescence where the indulged crystalline structure found to exhibit photo-response required for carrier generation as well as maintain the stability under light exposure owing to inclusion of small crystallites. The study will be useful in projecting the concept of higher solar efficiency with the effective way of light trapping with the use of such intrinsic absorber layer for solar cell designing.

Microwave Magnetic Resonance Absorption in U-Type Hexaferrite

Dubey, Divya Prakash¹, Kumar, Sandeep^{1,2} and Chatterjee, Ratnamala^{1*}

¹Magnetics and Advanced Ceramics Lab, Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016, India

²Department of Physics, Bhaskaracharya College of Applied Sciences, University of Delhi, Delhi-110075, India

Zn²⁺-Ti⁴⁺ substituted barium U-type hexaferrite polycrystalline samples: Ba₄Mn₂Fe_{36-2x}Zn_xTi_xO₆₀ (0.0 ≤ x ≤ 3.0, in steps of 1.0) have been synthesized by solid-state reaction method. The formation of desired U-type phase is confirmed by the X-ray diffraction (XRD) analysis. Further, the lattice parameters of the prepared samples were calculated by using Le bail refinement. The complex permittivity ($\epsilon^* = \epsilon' - i\epsilon''$) and permeability ($\mu^* = \mu' - i\mu''$) measurements were carried out on a Vector network analyzer (VNA, Agilent model PNA-L N5230A) in the microwave frequency range of 2-18 GHz. These parameters were used to calculate the reflection loss (R_L) in the samples and the minimum value of R_L was found at -29.51 dB for x=2.0 composition at 9.04 GHz frequency.

1. INTRODUCTION

The electromagnetic interference (EMI) has become a serious problem in the functioning of microwave (MW) devices which arises due to rapid development of MW communication systems used for defence and civil purposes. The MW absorbing materials can ease the problem of undesired MW signal by absorbing the incident MW energy and convert it into heat^[1]. Hexaferrites is the promising material for MW absorption as it offers simultaneous dielectric and magnetic loss in the single sample. Among all hexaferrite phases (M, Y, Z, W, X and U), the U-type Ba-hexaferrite (Ba₄Me₂Fe₃₆O₆₀), where Me is divalent transition metal ion, is most promising material to absorb MW in X-band frequencies (8-12 GHz) as it has large intrinsic magnetocrystalline anisotropy^[2]. In the present work, we have studied the effect on reflection loss (R_L) by the partial substitution of Fe³⁺ ions with Zn²⁺ and Ti⁴⁺ ions in Mn-U type hexaferrite and the reflection loss (R_L) results indicate the enhancement in the MW absorption after Zn²⁺ and Ti⁴⁺ ions substitution.

2.

EXPERIMENT

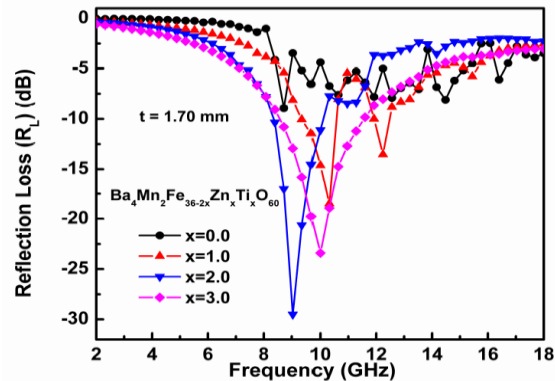
For the preparation of Polycrystalline samples of Ba₄Mn₂Fe_{36-2x}Zn_xTi_xO₆₀ through solid state reaction route, we have used BaCO₃ (99.9%), MnO (99.9%), TiO₂ (99.0%), ZnO (99.9%) and Fe₂O₃ (99.9%) starting raw materials. The complex permittivity ($\epsilon^* = \epsilon' - i\epsilon''$) and permeability ($\mu^* = \mu' - i\mu''$) were measured using vector network analyser (VNA) over 2-18 GHz frequency range. Naito and Suetake model^[3] was used to calculate input impedance Z_{in} of transmission line loaded with the sample of thickness (t) and given by,

$$Z_{in} = Z_0 \sqrt{\frac{\mu_r}{\epsilon_r}} \tanh\left(-\frac{2\pi j f t}{c} \sqrt{\mu_r \epsilon_r}\right) \quad (1)$$

The reflection loss (R_L) was calculated using the formula

$$R_L(dB) = -20 \log_{10} \left(\frac{Z_{in} - Z_0}{Z_{in} + Z_0} \right) \quad (2)$$

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Effect of partial absence of hydrogen on graphene quality during CVD graphene growth

Sharma, Indu*, Subhedar, Kiran M and Dhakate, Sanjay R

Advanced Carbon Products, Advanced Materials and Devices Division, CSIR-National Physical Laboratory (NPL), New Delhi-12, India.

**E-mail of Corresponding Author: indusharma.86@gmail.com*

ABSTRACT

Dual performance of hydrogen makes it important in growth of graphene by CVD method. Hydrogen acts as both activator as well as etchant during growth of graphene. Nucleation centres during growth process can be controlled by playing with hydrogen flow rate. In present work, presence and partial absence of hydrogen during pre-annealing process and its effect on graphene quality is studied. Absence of hydrogen for few minutes before growth of graphene partially oxidizes surface of copper foil suppresses the nucleation density of graphene and this step improves the quality of graphene. After growth, graphene was transferred on SiO₂ substrate and were characterized using optical and Raman spectroscopy.

Liquid Phase Exfoliation of bulk Molybdenum Disulfide in 2D Sheet and its application in mobility enhancement of Poly (3-hexylthiophene-2, 5-diyl)

S.P. Tiwari^a, Md. B. Alam^b, Razi Ahmad^c, C.K. Suman^d, Ritu Srivastava^e
*Advance Material Devices Division, CSIR-National Physical Laboratory, Dr.
K.S.Krishnan Road, New Delhi-110012, India
Email: suryatiwari04el@gmail.com*

The free standing few-layered flakes of molybdenum disulfide (MoS₂) have been obtained by liquid phase ultrasonicated exfoliation of bulk MoS₂ powder in Ortho di chlorobenzene. The as exfoliated nanoflakes were characterized by UV-Vis absorption spectroscopy and Atomic force microscopy (AFM). The thickness and lateral size of the flakes was calculated from the AFM. The AFM height profile of exfoliated MoS₂ flakes showed height of 7 nm, showing few layer of flakes. This indicate that liquid phase exfoliation method can be used to produce large quantities of two-dimensional layers of MoS₂ and can be used for photovoltaic cell and optoelectronic devices. Exfoliated MoS₂ nano sheets have been dispersed in P3HT and OFET has been fabricated to calculate it's linear as well as saturation mobility. P3HT polymer has not adequate mobility for switching device application, by mixing the MoS₂ nanosheets in P3HT solution, mobility is enhanced from **1.48×10⁻¹ cm²/V-s** to **2.71×10⁻¹ cm²/V-s**.

Theory for Work Function of Curved Metal Nanostructures

Kaur, Jasmin and Kant, Rama
Complex Systems Group, University of Delhi,
Department of Chemistry, New Delhi-110007, India
*Email: jasminkaur80@yahoo.in, *rkant@chemistry.du.ac.in*

We present an analytical theory for the electronic work function in curved metal geometries under Thomas–Fermi approximation¹. The work function is framed as the work against the electrostatic self-capacitive energy of a circular disc of radius of Thomas-Fermi electronic screening length¹. The curvature contributions are accounted by the mean and Gaussian curvature (through multiple scattering expansion)^{2,3}. The anomalous variation in work function of metal and semimetal nanostructures is shown to arise when the surface radius of curvature is in units of the electronic screening length. Theory predicts an anomalous enhancement in the work function of spherical nanoparticles. The effect of shape anisotropy is illustrated through ellipsoidal particles which exhibit non-uniform distribution of work function over the surface. The maximum value of work function is observed at the equator and poles for oblate and prolate particles, respectively, whereas triaxial ellipsoid shows nonuniform distribution of the work function over the surface. The theory predicts manifold increase in the work function for a particle with sub-nanometer scale roughness. Similarly, the electronic work function of a wet electrode is generated through inclusion of the contribution from the first layer of solvent dipoles^{4,5}. Theory shows that the effect of solvation of an electrode is manifested as the decrease in its work function⁴. The anomalous variation in work function for nanostructured electrode is manifested due to its shape and size. Finally, the theory is validated with experimental data, and it is concluded that the work function of a nanoparticle can be tailored through its shape.

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