1ST International e-Conference on

Recent Advances in Physics & Materials Science-2020

(IC-RAPMS-2020)

July 9 - 10, 2020 (10:00 AM- 02.00 PM, IST)

Organized by

Kurseong College, Darjeeling, West Bengal, India-734203

In collaboration with

St. Joseph's College, Darjeeling, West Bengal, India-734104

Technical partner

Condensed Matter Physics Research Center, Butwal, Nepal-11

Abstract Book

Theme

- *Energy Materials*
- *Nano and Biomaterials & Applications*
- *Crystal Growth & Applications*
- *Organic & Inorganic materials*
- *Magnetic Materials and Spintronics*
- *Solar Energy, Thin Films*
- *Mathematical Modeling*
- *Liquid Crystal & Solar cell*
- *Soft Condensed Matter*
- *Particle and Nuclear Physics*
- *Astrophysics and Space Research*
- *Polymers and Composite Materials*

Speakers

Sl. No.	Name	Institute/University	Title of Talk
1.	Prof. V. Madhurima	Central University of Tamil Nadu, India	Droplets: Properties and Relevance to COVID -19
2.	Dr. D.P. Rai	Pachhunga University College, India	Thermoelectric properties of Heusler alloys
3.	Dr. M.P. Ghimire	Tribhuvan University, Nepal	Creating Weyl nodes by Magnetization Rotation in Kagome Metal $Co_3Sn_2S_2$
4.	Dr. Arles V. Gil Rebaza	Instituto de Física La Plata IFLP – CONICET, CCT, Argentina	The GIPAW approach for the study of local structures and the electric field gradients at Cd and Ta impurity sites. Application to doped yttria ceramics
5.	Dr. Debarun Dhar Purkayastha	NIT-Nagaland, India	Thin Films and Nanostructures for Self-cleaning Applications
6.	Dr. Anand Pariyar	Sikkim University, India	Metal organic framework as functional materials
7.	Prof. B. Indrajit Sharma	Assam University, India	Density Functional Theory: electronic structure calculation
8.	Dr. P.K. Das	University of Oslo, Norway	Minerals behavior under extreme conditions: A DFT approach
9.	Dr. D. Gupta	Weizmann Institute of Science, Israel	Charged particle collisions and its implications to atomic and molecular systems
10.	Dr. P. Pradhan	MIT Kavli Institute for Astrophysics and Space Research, USA	Astrophysics, neutron stars and animals. Wait, what?
11.	Prof. P. Poulose	IIT Guwahati, India	Cosmic Evolution and Particle Dynamics
12.	Dr. Pratap Reddy	National Institute of Nutrition, Hyderabad, India	In vivo imaging in nanoparticles based drug delivery to target tumor- an advanced and accelerating biomedical imaging method
13.	Prof. Y. Al-Douri	University of Malaya, Malaysia	Quantum dots: Theoretical studies
14.	Dr. Debasish Borah	IIT Guwahati, India	Neutrinos at the crossroads of particle physics, astrophysics and cosmology

Table of content

55	Bishnu Karki, Bishnu Prasad Belbase and Madhav Prasad Ghimire Email: bishnukarki724@gmail.com	Novel Topological Weyl Semimetallic Phase in layered material: Fe2Sn	81
56	Debopriyo Ghoshal, Debopriya Bhattacharya, Dheeraj Mondal, Sukhen Das, Navonil Bose and Mousumi Basu Email: navonil05@gmail.com	Bromothymol Blue Dye/ PVA composite films: Facile economic and flexible laser filters	82
57	Smita Rai, Nayan Sharma and Dhurba Rai Email: smitarai030@gmail.com	Structured water chains in external electric fields	84
58	Subhrajyoti Biswas Email: anjansubhra@gmail.com	Consequences of pi-eta mixing in nuclear matter	85
59	Daya Nidhi Chhatkuli, Sanjaya Paudel and Binil Aryal Email: chhatkulidn@gmail.com	A Spectroscopic study of the Low Redshift Dwarf Galaxy SDSS J134326.99+431118.7 to Calculate Star Formation Rate	86
60	Dhurba Raj Jaishi and Madhav Prasad Ghimire dhurbajaishi2019@gmail.com	Study of Electronic, Magnetic and Transport properties of BaTbO3	87
61	R. K. Rai , G. C. Kaphle and O.P. Niraula Email: rairajk@gmail.com	First-principle Study of Electronic Structures of Complex Transition Metal Oxides: CaVO3/SrVO3	88
62	Gang Bahadur Acharya and Madhav Prasad Ghimire Email: acharyagangbdr@gmail.com	Identification of half metallicity in Co-doped Rb2Ni3S4	90
63	Haripriya Rath, U.P. Singh and N.C. Mishra Email:haripriyarath@gmail.com	Effect of thermal annealing on Structural and micro structural property of DC sputtered TiO2 thin film	91
64	Ayan Banik Email: ayanbanik97@yahoo.com	High-Performance Thin Film Solar PV Technology in Context to Indian Energy Sector	92
65	Rajmoni Basumatary and Anjalu Ramchiary Email: onjalu@gmail.com	Synthesis and characterization of visible light active TiO2/CoTiO3 hybrid nanostructure and study of its charge carrier transfer dynamics	93
66	Samiran Upadhyaya, Saponjeet Borah and Neelotpal Sen Sarma Email: samiranupadhyaya@gmail.com	Biosynthesis of Gold Nanoparticles by using the aqueous leaf extracts of Elaeocarpus serratus	94
67	Varun D. Sharma and Milan Kumar Bera Email: m.k.bera@mmumullana.org	Recent advances in fluorescent carbon quantum dots for white LED applications	95
68	Kheyali Barman, Rajashree Nath, Arnab Sen, Bakul Das, Sujay Pal and Prabir Kr Haldar kheyalibarman.dth@gmail.com	Monitoring of Geomagnetic storm induced VLF signal disturbances from a Low Latitude Station at Cooch Behar, India	96

69	K. Manjunatha, V. Jagadeesha Angadi and U. Mahaboob Pasha Email: jagadeeshbub@gmail.com	Bismuth doped Cobalt Chromates nanoparticles: A detailed study of Structural, Microstructural, Electrical and Magnetic Properties	98
70	Indrajit Ghosh, Sukhen Das and Nabajit Chakravarty Email: indraghosh06@gmail.com	Stellar Scintillations and Occultation: An Astrophysical Approach to the Guiding Turbulence in Tropical Cyclones	100
71	Monoj Das and Bikash C Gupta Email: dsmonoj@gmail.com	Diameter and atomic structure dependent structural and electricalproperties of zigzag ZnTe nanotubes	102
72	Amitabha Bhattacharyya Email: abhattacharyya@cus.a	The Science Behind the Unsung Indian Musical Drums	104
73	Nakul Chhetri, Amit Shanker, PK Mandal and PC Barman Email: nakulgorkha@gmail.com	Investigation of ground state properties of ternary chalcopyrite, CuXY2(X=Al, Ga,In; Y=S,Se)using DFT	105
74	Nileema Sharma and Madhav Prasad Ghimire nileemasharma012@gmail.com	Flat band and half metallicity in Kagome magnet $Y_{1-x}Ca_xCo_5$	106
75	Nirmal Saud and Madhav Prasad Ghimire Email: saud.nirmal05@gmail.com	Electronic and Magnetic properties of BiTeI	107
76	Labanya Ghosh1 and Sandip Chatterjee Email:labanya.ghosh1@gmail.com	Consequences of Ni Doping on Thermoelectric Properties of Bi_2Te_3	108
77	Sarita Lawaju, Shalika Ram Bhandari and Madhav Prasad Ghimire sarita.lawaju0106@gmail.com	Electronic and Magnetic Properties of Double Perovskite Tb_2FeCrO_6	109
78	Neetu Sharma, Indu Sharma, Tulshi Chakraborty and Milan Kumar Bera Email: m.k.bera@mmumullana.org	Naturally derived biocompatible fluorescence carbon quantum dots for in vivo targeting and imaging of tumor cells	110
79	Shivani Chaudhary Email: shivanilko810@gmail.com	DFT study of Liquid Crystal materials	11
80	Shyam Sundar Sharma Email: shyam14u27@gmail.com	The Study of Structural and Dynamical Properties of Heavy Water (D2O) Passing Through Carbon Nanotubes	112
81	U. J. Vedash, Surinder Singh and Sushil Kumar Kansal Email: sonuunos@gmail.com	Ecofriendly zirconium MOF and graphene based nanohybrid for degradation of pharmaceutical drug from wastewater	113
82	Anirban Das Email: anirban.mintu@gmail.com	Study of deformation behaviour of metallic nanowires by using multi-scale computational modelling	114
83	Subhabrata Senapati, Aunggat Shah, Mrityunjoy Mahato and P. K. Patra Email: mrityunjoyphy@gmail.com	Indirect Calculation of Elastic Modulus of CNT Composites	116
84	Sudeep Jnawali and Madhav Prasad	Electronic properties of topological	

DEFORMULATION AND CHARACTERIZATION STUDIES OF REFERENCE DRUG PRODUCT CONTAINING ETORICOXIB

S. Jailani[1] and C.K. Dhanapal[1]

[1] *Dept. of Pharmacy, Annamalai University, Chidambaram, Tamil Nadu.*

(Research Area: Material Characterization)

Abstract: Etoricoxib, is a relatively advanced drug for treatment of pain with improved safety features. The marketed innovator drug product formulation was systematically subjected reverse engineering studies involving material characterization studies and instrumental analytical evaluation to decode the information related drug physicochemical information related critical material attributes and to decide the tentative qualitative and quantitative composition. The characterization studies and the outcome is very important input information in designing and development of generic drug product for improved cost effectiveness and availability of economical drug product availability in the market for enhanced accessibility in developing countries.

ESTIMATION OF RADON AND THORON EQUILIBRIUM FACTORS IN INDOOR ENVIRONMENT USING NUCLEAR TRACK DETECTORS

A. Pyngrope[1], A. Khardewsaw[1], Y. Sharma[2], D. Maibam[3], A. Saxena[1] and B. K Sahoo[4]

[1]Department of Physics, North-Eastern Hill University, Shillong
[2]Department of Physics, Don Bosco College, Tura
[3]Don Bosco College of Teacher Education, Tura
[4]Radiological Physics and Advisory Division, BARC Mumbai

(Research Area: Particle and Nuclear Physics)

Abstract: Radon (^{222}Rn) and its isotope thoron (^{220}Rn) are mobile, chemically inert and radioactive gaseous elements that are produced spontaneously during the decay process of radium isotopes from Uranium (^{238}U) and Thorium (^{232}Th) respectively. Usually, these gases tend to accumulate inside enclosed spaces like underground mines and residential dwellings. Radon and thoron together with their short-lived progeny (^{212}Po and ^{214}Po) contribute about 52 % of the natural sources of radiation exposure to mankind. It has been reported that, progenies are mainly responsible for inhalation dose due to their particulate nature. Since, measurement of progeny is difficult, the equilibrium factor is used as a proxy for the progeny and is also a factor used in the calculation of Working Level Month (WLM), Annual Effective Dose (AED) etc. The equilibrium factor (f) is actually the ratio of the Equilibrium Equivalent Concentration (EEC) to the Radon/Thoron (C_R or C_T) activity concentrations, typically expressed as:

$$f = EEC/(C_R \text{ or } C_T) \quad (1)$$

The present study reports the estimate of equilibrium factors from the measured activity concentration of radon, thoron and their progeny in different dwelling types under East Khasi Hills district of Meghalaya, India. Single entry pin-hole dosimeter and Direct radon/thoron progeny sensors have been used for the measurement methodology with LR-115 type II film as detector. Tracks formed on these detectors are converted to the individual activity concentration of indoor parameters using standard calibration factors. Results showed that both radon (f_r) and

thoron (f_t) equilibrium factors in concrete (viz, f_r = 0.41, f_t = 0.023) and semi-concrete structures (viz, f_r = 0.42, f_t = 0.022) have comparable values, while wooden structure (viz, f_r = 0.36, f_t = 0.020) witnessed comparatively much lower values. Overall, the reported *f* - values seem to be in the range as those reported elsewhere and also found to be comparable with those given by UNSCEAR, which is 0.4 for radon and 0.1 for thoron.

NUSTAR AND SWIFT OBSERVATIONS OF X-RAY BINARY 4U 1901+03

Binay Rai[1]

[1]*Department of Physics, University of North Bengal, Darjeeling, West Bengal*

(Research Area: Astrophysics and Space Science)

Abstract: We studied the spectral and timing properties of 4U 1901+03 using NuSTAR and Swift observations during recent outburst. Large number of flares were observed in the light curves varying from tens to hundreds of seconds. Pulse profiles were varying with both time and energy. At the beginning of an outburst the pulse profile was single peaked which evolved into double peaked to a single peaked again. These variation of pulse profiles is possibly due to transition of the pulsar from one to other accretion regime. The pulse fractions of the pulsar were found to increase with an increase in energy. We simultaneously fitted Swift and NuSTAR spectra in a 0.5-79 keV energy range using CUTOFFPL and GAUSSIAN models, an absorption like feature near 10 keV were observed in the residue of the fitted spectra, so we incorporated another model GABS in order to account for this absorption like feature. This feature were found to show positive correlation with luminosity, it also depends on pulse phase. The dependence of this feature on the luminosity and pulse phase indicates the fact that this feature can be none other than cyclotron resonance scattering feature (CRSF) . However this 10 keV feature is observed in other pulsars having CRSF or not and also shows phase dependence which raises a doubt for this feature to be CRSF in our observations, it is equally possible that it is due to limitation of our continuum models used in fitting the spectrum.

BUCKLING ANALYSIS OF NONUNIFORM NANOBEAMS USING NONLOCAL ELASTIC THEORY AND DIFFERENTIAL TRANSFORMATION METHOD

B. R. K. L. Lyngdoh Mawphlang[1] and P. K. Patra[1]

Department of Physics, North-Eastern Hill University, Shillong 793022, India

(Research Area: Nano and Biomaterials & Applications)

Abstract: Nanobeams exhibit greater strength compared with larger structures due to a reduction in the number of defects per unit length. This idea is supported by the fact that there is an increase in strength of a nanobeam with decreasing diameter. However, they show buckling behaviour under axial compression due to their slenderness. This limits their use in applications. Although extensive studies have been done to understand buckling behaviours of uniform nanobeams, the study is limited for nonuniform nanobeams. Keeping view a wide applications of nonuniform nanobeams such as tips of AFM, STM, etc., it is important to study their buckling behaviours before their uses.

The classical elastic theory is quite reliable to analyse the buckling behaviour of large length scale nanobeams, but it is questionable at very small length scale because it does not take into account the important contributions of material microstructure, such as lattice spacing between individual atoms. In this paper, we have used a nonlocal elastic theory to capture the effect of small scale parameter on the buckling behaviour of nonuniform nanobeams. The governing differential equation for nonuniform nanobeam subject to the axial compressive load is derived. The numerical solutions are obtained using the differential transformation method (DTM). It is found that the effect of small scale parameter on the buckling load of both uniform and nonuniform nanostructures is significant that cannot be ignored. Our solutions are in good agreement with that of the analytical solutions for uniform nanobeam. This shows that the DTM can be used as an important mathematical tool to analyse the buckling behaviour of nonuniform nanobeams with various boundary conditions.

Keywords: Nonlocal elastic theory, buckling behaviour, small-scale effect, differential transformation method.

References:

[1] H. B. Khaniki, S. H. Hashemi, *Eur. Phys. J. Plus* 132, 500 (2017).

[2] A. C. Eringen, *J. Appl. Phys*. 54, 4703 (1983).

[3] A. Arikoglu, I. Ozkol, *Appl. Math. Comput.* 168, 1145 (2005).

DENSITY FUNCTIONAL STUDIES ON STRUCTURAL, ELECTRONIC AND MAGNETIC PROPERTIES OF Rhn (n = 9–20) CLUSTERS

Abhijit Dutta[1]

[1]*Department of Chemistry, North-East Junior College, Assam*

(Research Area: Nano Materials)

Abstract: Methodical exploration is performed on Rh*n*(*n* = 9–20) clusters in the gas phase with all electron relativistic methods usingdensity functional theory (DFT) within the generalized gradient approximation. Neutral clusters with even atoms of rhodiumand ionic clusters containing odd atoms of rhodium are optimized with odd multiplicities, while neutral clusters containingodd rhodium atoms and ionic cluster having even atoms of rhodium are optimized with even multiplicities. DFT-based structuraland reactivity parameters such as stability function, dissociation energy, HOMO–LUMO gap, ionization potential andelectron affinity reveal higher stability of Rh_{13},$Rh_{14}$and Rh_{19}clusters. Among these clusters, icosahedral $Rh_{13}$is obtained tobe the most stable. Magnetic moment and spin density analysis suggest nonzero magnetic moment for all clusters. Rh_{13} and $Rh_{14}$are found to have higher activity towards O–H activation. Ruthenium-dopedrhodium clusters have also been utilized to investigate the reactivity and catalytic activity of the same reaction and found toexhibit higher activity. Among all alloy clusters, Rh_{18}Rudissociates O–H more easily.

OAT-g-PAM: SYNTHESIS, CHARACTERIZATION & APPLICATION AS AN ADHESIVE

Srijita Bharti[1]

[1]*Department of Chemistry, Cambridge Institute of Polytechnic-Baheya, Angara, Ranchi, Jharkhand, India.*

(Research Area: Polymers and Composite Materials)

Abstract: Various grades of polyacrylamide grafted oatmeal (OAT-g-PAM) were synthesized via '*conventional'* grafting technique. Synthesis was optimized by changing monomer and CAN concentration for all the grades. The grafting reaction was confirmed using number average molecular weight, solubility and ^{13}C-CP/MAS Solid-state NMR spectroscopy. The grafted biopolymers were assessed for its application as impending adhesive by fabricating a single lap joint of two wood blocks. Adhesivewere subjected to check its mechanical behaviorup tofailure or breaking. The breaking point of the joint was determined using a universal testing machine (UTM) after curing as per protocol. The objective of this research is to characterize the behavior of the synthesized novel adhesive under different compression shear loads. Adhesion characteristics of synthesized OAT-g-PAM adhesive were compared with a commercially available adhesive using similar test conditions in which performance of the best optimized grade was found superior than that of commercially available adhesive.

Keywords: oatmeal, graft copolymers,adhesive,^{13}C-CP/MAS Solid-state NMR spectroscopy, universal testing machine.

POLYELECTROLYTE COMPLEX NANOPARTICLES AS EFFICIENT MATERIAL FOR PROTEIN SENSING

Hrishikesh Talukdar[1] and Sarathi Kundu[1]

[1]*Department of Physics, Assam Engineering College, Jalukbari, Guwahati-13, Assam, India*

(Research Area: Nano and Biomaterials and applications)

Abstract: Hyperalbuminemia or hypoalbuminemia are conditions which occur due to the quantitative variation of albumin protein in human body and causes inflammation of liver, bone marrow disorder, chronic hepatitis, kidney disorder, etc. Various experimental methods have been developed to improve the protein detection method; however, sensitivity still remains a major issue. Therefore, there is a need to develop a better sensitive and cost-effective method in order to avoid different protein related diseases. In this work we have prepared polyelectrolyte complex nanoparticle (PECNP) using two commercially available polyelectrolytes poly(Na-4styrene sulfonate) (PSS) and poly(diallyledimethyleamoniumchloride) at molar mixing ratio (n-/n+) of ≈ 0.4, 0.67, 0.75 and 1.5 by applying consecutive centrifugation to modify the optical property of PSS. However, for n-/n+ ≈ 0.75, PEC NPs exhibit larger blue-shift and specific emission peak occur at ≈ 278 nm for the 225 nm excitation. The emission peak intensity of PECNP is quenched in presence of very low concentration (≈ 5 nM) of human serum albumin and lysozyme protein. The quenching increases linearly with increasing protein concentration which can be attributed by the Förster resonance energy transfer (FRET) as protein absorption also occurs at 278 nm due to tryptophan residue. The FRET is established by calculating the separating distance between donor and acceptor which varies between 1 and 3 nm. Therefore, the modified emission behavior of synthesized PECNP can be used as promising and efficient material for protein sensing. The other characterization related to particle formation and conformation is done using AFM, TEM and FTIR.

EFFECT OF POROSITY AND NON-LATTICE OXYGEN ON RESISTIVE SWITCHING IN Nb_2O_5-BASED THIN-FILM DEVICES

Karimul Islam[a,b], Rezwana Sultana[a,b], Abhishek Rakshit[a,b], U. K. Goutam[b], Supratic Chakraborty[a]

[a]*Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Kolkata 700 064, India*

[b]*Homi Bhabha National Institute, BARC Training School Complex, Anushaktinagar, Mumbai 400 094, India*

Abstract: Niobium pentoxide (Nb_2O_5) thin-films were deposited on n-type Si substrates using dc reactive sputtering at various O_2/Ar ratios. X-ray reflectivity (XRR) and synchrotron-based X-ray photoelectron spectroscopy (XPS) facilities were employed to determine the film thickness, surface morphology and oxidation states of the as deposited samples. Al /Nb_2O_5/Si metal–insulator–semiconductor (MIS) devices were fabricated to study their resistive switching phenomenon. In the manuscript, an attempt has been made to investigate the role of porosity of Nb_2O_5 films on the switching properties of Nb_2O_5-based MIS devices. The current vs gate voltage (I-V) plot display sharp transition in current (~ up to five orders) denoting a switching between high resistance state to low resistance state. XRR profiles of deposited samples were fitted using parratt formalism to get film thickness and electron density profile. Surface and interface roughness of the films were also estimated from the fitted curves. The XPS spectra of Nb 3d and O 1s of all the samples are deconvoluted using PeakFit 4.11 software. The analysis of peak positions in Nb3d spectra, indicates formation only of Nb_2O_5 oxides whereas O1s spectra ensures presence of lattice and non-lattice oxygen in all thefilm. The percentage of non lattice oxygen was estimated from XPS curves. Non lattice oxygen influences the switching phenomenon. Film porosity also plays a vital role in determining the on/off ratio. Therefore porosity of the films along with oxygen vacancies determines the switching properties of sputter deposited Nb_2O_5 thin films.

PREPARATION OF MRI/NIR-II MULTIMODAL IMAGING AGENT BASED ON BIO-COMPATIBLE SILVER CHALCOGENIDE QUANTUM DOTS.

Karishma Bhardwaj[1] and Sudarsan Tamang[1]

[1]*Department of Chemistry, Sikkim University, Gangtok, Sikkim, India*

(Research Area: Nano and Biomaterials and applications)

Abstract: Bio-compatible, nontoxic colloidal quantum dots with absorption/emission properties in the second near infrared region (NIR-II, 1000-1400) are highly desirable for optical imaging and biosensing due to increased signal-to-noise ratio in the wavelength window. Highly aqueous stable silver chalcogenide quantum dots offer a non-toxic and stable alternative to existing Pd, As, Hg and Cd-based NIR-II colloidal quantum dots (CQDs). The talk will focus on the practicable access to NIR-II emission windows with Ag_2X (X=S, Se) CQDs using thio/selenourea precursors and their analogues. These colloidal quantum dots (size < 5 nm) are then aqueous phase transferred with high retention of fluorescence quantum yield (~5 %) and good colloidal stability. Finally, we will demonstrate the method of preparation of a multimodal NIR-II/MRI contrast agent with tunable fluorescence and high T_1 relaxivity (407-990 mM^{-1} s^{-1} per QD).

DYNAMIC PROPERTIES OF NEW HALF-METALLICMn_2ScZ (Z = Si, Ge and Sn) HEUSLER ALLOYS

M. Ram[a,b*], A. Saxena[b], H. Joshi[a,c], A. Shankar[a]

[a]*Condensed Matter Theory Research Lab, Department of Physics, Kurseong College, Darjeeling, India-734203.*

[b]*Department of Physics, North-Eastern Hill University, Shillong, India-793022.*

[c]*Department of Physics, St. Joseph's College, North Point, Darjeeling, India-734104.*

(Research Area: Theoretical Condensed Matter Physics)

Abstract: The ground state structural and mechanical stability along with the half-metallic nature of new Mn_2ScZ (Z = Si, Ge and Sn) Heusler alloys using first principal calculations was established in our previous paper [1]. In this paper, we have reported the dynamical stability and properties of above mentioned Heusler alloys. The phonon dispersion curve was obtained using two different methods namely, density functional perturbation theory as implemented in Quantum ESPRESSO [2] and finite displacement method as implemented in Phonopy [3]. The longitudinal and transverse elastic sound velocities were also determined and the directional components of these velocities were found to correlate with the spatial dependence of elastic moduli as obtained from ELATE [4].

Reference:

[1] M. Ram, A. Saxena, Abeer E. Aly and A. Shankar, *RSC Adv.* **10** 7661 (2020).

[2] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti. M. Cococcini, I. Dabo and A. Dal Corso, *J. Phys.: Condens. Matter.* **21** (2009).

[3] A. Togo and I. Tanaka, *Scripta Materialia*, **108** (2015).

[4] R. Gaillac, P. Pullumbi and F.X. Coudert, *J. Phys.: Condens. Matter,* **28** (2016).

A COMPARATIVE ANALYSIS OF ALL FIBER OPTIC SENSORS FOR DETECTION OF ADULTERATION IN FOSSIL FUELS

Mukesh Pradhan[1]

[1]*Tufanganj Mahavidyalaya, Suknirpar Dham, Andaran Phulbari, West Bengal-736159, India*

(Research Area: Electronics)

Abstract: Refractive index is directly proportional to the concentration of medium. Based on thisprinciple, we report two schemes of measuring varying concentration of solvent by measuringoutput response through intensity interrogation. In the first case, we use evanescentfield by exposing certain portion of a cladding to varying concentration of fossil fuels. Inthe second case, we utilize reflectance through a displacement scheme for measuring thesame analyte. Accordingly, all results are comprehensively analyzed and all sensing performancesare procedurally investigated. The sensitivity of both the schemes are estimatedand compared. The evanescent fiber optic set-up renders better response as compared tothe displacement one. Due to simplicity in design approach, the all fiber optic schemesprove to be highly adaptable to sense other chemical contaminants.

REDUCED GRAPHENE OXIDE CONTAINS A MINIMUM OF SIX OXYGEN ATOMS FOR HIGHERDIPOLAR STRENGTH: A DFT STUDY

Narinder Kumar[1]

[1]*Department of Physics, School for Physical & Decision Sciences, Babasaheb Bhimrao Ambedkar University, Vidya Vihar, Raebareli Road, Lucknow, India.*

(Research Area: Condensed Matter Physics and Material Science)

Abstract: The present work focused on the reduced graphene oxide contains a minimum of six oxygen atomsfor the higher dipolar strength. The ionization potential and electron affinity decreased only for thesix oxygen atoms based graphene. The six oxygen atoms based graphene have the highest dipolemoment. The reduced graphene has 0.25 eV bandgap, which is very suitable for electron transfer.The six oxygen atoms based graphene leads to the least gauge including atomic orbital (GIAO)rotational tensor; however, it has the highest isotropic polarizability difference, diamagneticsusceptibility tensor difference, paramagnetic susceptibility tensor difference, and total susceptibility.The C-C bond length has increased only for the six oxygen atoms based graphene

Keywords: Reduced graphene oxide, Doping of oxygen atom, DFT (B3LYP), Bandgap, Magneticproperties.

ANALYSIS OF THE EFFECT OF LOAD DIRECTION ON THE STRESS DISTRIBUTION IN ORTHOPAEDIC IMPLANTS

Nihar R Mahapatra[1], Manit Gosaliaiv[1], Ishika Tulsian[1]

[1]*Department of Physics, Aditya Birla World Academy, Mumbai, India*

(Research Area: Nano and Biomaterials and applications)

Abstract: Orthopaedic implant materials have an important role in the field of medical science. Characteristics of implant materials such as rigidity, corrosion, biocompatibility, surface morphology, tissue receptivity, and stability are the key factors that influence the choice of the implant material. Mechanical properties of the implants are one of the significant factors for a bone substitution. To understand the mechanical properties of these solid substitutes, the use of solid mechanics, which is intended for general structural analysis of 2-dimensional and 3-dimensional bodies is vital. In this study, 3-dimensional modelling of implant and simulation using the finite element analysis software were incorporated to investigate the effect of load direction on the stress distribution in different orthopaedic implant materials.

NUMERICAL SIMULATION ON BIOCONVECTION OF NANOMATERIAL IN POROUS MEDIA ALONG A VERTICAL PLATE

Pinaki Pal[1] and Asish Mitra[2]

[1]*Department of Physics, M B B College, Agartala, Tripura, India*
[2]*Department of Physical & Material Sciences, College of Engineering & Management, Purba Medinipur, West Bengal, India*

(Research Area: Nano and Biomaterials and applications)

Abstract: Bioconvection is one of the rapidly growing fields in science combining thermal physics, hydromechanics and biology. Bioconvection is the directed flow of microorganisms in a liquid medium. In the present numerical simulation, steady, laminar, two-dimensional natural bioconvective nanomaterial flow along a vertical plate in the presence of motile microorganisms is investigated. The plate is embedded in a saturated Darcy porous medium and subjected to surface heat flux, nanoparticle volume fraction and motile microorganisms fluxes. Here nanofluid is nanomaterial and Boungiorno model is employed that treats the nanofluid as a two-component mixture (base fluid plus nanoparticles), incorporating the effects of Brownian motion and thermophoresis. By appropriate similarity variables, the governing nonlinear partial differential equations of flow are transformed to a set of nonlinear ordinary differential equations. Subsequently they are reduced to a first order system and integrated using Newton Raphson and adaptive Runge-Kutta methods. The computer codes are developed for this numerical analysis in Matlab environment. Dimensionless stream function (s), longitudinal velocity (s'), temperature (θ), nanoparticle volume fraction (f) and motile microorganism density profile (ξ) are computed and illustrated graphically for various values of the pertinent dimensionless parameters, namely, bioconvection Lewis number (Lb), Lewis number (Le), bioconvection Peclet number (Pe), buoyancy-ratio parameter (Nr), bioconvection Rayleigh number (Rb), Brownian motion parameter (Nb), thermophoresis parameter (Nt) and power-law

variation index (λ). The results obtained from the present simulation are in with good agreement with the previous reports available in literature.

Keywords: Bioconvection, Motile Microorganisms, Natural Convection, Nanofluid, Vertical Plate.

STATISTICAL PROPERTIES OF ACTIVE PARTICLES

Prashant Singh[1]

[1]*International Centre for Theoretical Sciences (ICTS-TIFR)*

(Research Area: Condensed Matter Physics)

Abstract: Active matter is a class of particles that are driven at the individual level by consuming energy from surrounding. The dynamics of this particle is liberated from the constraint of time-reversal symmetry which takes them beyond the ambit of statistical mechanics. This liberation, in addition, gives rise to a plethora of interesting features which are otherwise not observed. The list includes- ocking in birds, school of sh, chemotaxis in bacteria and so on. Apart from the interesting emergent behaviours, the self-propelling nature of these particles makes them quintessential candidates in nano-technology as micro- motors, cargo carriers, drug transports, ratchet e ects. In this talk, I will introduce the active matter and then present the results on probability distribution, persistent properties, rst passage distributions for this system.

References

[1] Kanaya et al, arXiv:1711.08474.

[2] Prashant et al, arXiv:1906.09442, arXiv:2004.11041.

UNDERSTANDING ASYMMETRY IN ELECTROMAGNETICALLY INDUCED TRANSPARENCY FOR 87-Rb IN STRONG TRANSVERSE MAGNETIC FIELD

Indra Hang Subba[1], Ranjit Kumar Singh[1], Nayan Sharma[1], Souvik Chatterjee[1] and Ajay Tripathi[1]

[1]*Department of Physics, Sikkim University, Tadong, Gangtok, Sikkim, India*

(Research Area: Laser and Quantum Optics)

Abstract: We present the results of our experimental investigation performed for D_2 line of 87-Rb. In thiswork, we have studied the phenomenon of electromagnetically induced transparency of 87-Rb in presenceof a transverse magnetic field and it is interesting to find the EIT spectrum shows signature of the closelylying hyperfine excited states in particular F' = 1. We choose two different configurations for our studynamely, $\Lambda_1$and$\Lambda_2$realized by locking probe beam at two different transitions. We observe asymmetric features in both configurations at highmagnetic field and for Λ_1 configuration we find complete conversion from transmission toabsorption. We explain the observations by quantitative assessment of the impurities in thedark states which arises because of the influence of the neighboring states. At high magnetic field, population realignment among Zeeman sub-levels becomes prominent. We substantiate ourexperimental findings with density based numerical calculations.

INFLUENCE OF Zr CONCENTRATION AND RELEASE OF LATTICE OXYGEN ON RESISTIVE SWITCHING OF $Zr_xHf_{1-x}O_2$– BASED METAL-OXIDE-SEMICONDUCTOR DEVICES

Rezwana Sultana[a,b], Karimul Islam[a,b], Abhishek Rakshit[a,b], Manabendra Mukherjee[a] and Supratic Chakraborty[a]

[a]*Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Kolkata 700 064, India*

[b]*Homi Bhabha National Institute, BARC Training School Complex, Anushaktinagar, Mumbai 400 094, India*

Abstract: In this work we investigate the effect of Zr concentration on memory performance of co-sputtered deposited $Zr_xHf_{1-x}O_2$-based metal-oxide-semiconductor (MOS) devices. $Zr_xHf_{1-x}O_2$ thin-films are deposited at different powers to Zr target keeping RF power to HfO_2target fixed. Then 150 nm thick Al film is evaporated on the deposited film using electron beam evaporation system. Finally the top metal film is patterned to 100 μm-diameter gate electrodes by UV photolithography to construct MOSdevices.The electrical characterization and x-ray photoelectron spectroscopy (XPS) study brings out that the resistive switching is maximum whenZr concentration in the film is 9.11%. XPSalso reveals presence of non-lattice oxygen in the oxide layer of all the devices. The differential scanning calorimetry (DSC) study exhibits an endothermic peak at ~ 145.9 °C only for that specific sample that contains particular Zr concentration in the $Zr_xHf_{1-x}O_2$ film indicating release of lattice oxygen.Hence, besides presence of non-lattice oxygen in the oxide film, generation of hole trap density in the form of lattice oxygen release is also responsible to produce a better low resistance state (LRS). The double logarithmic plot of I-V measurement agrees the same. At certain higher temperature the released lattice oxygen is reversibly turned around to their respective previous positions that helps to gain high resistance state(HRS). This may happen due to the one kind of micro structural arrangements at a critical Zr content that offer the lowest resistive state of the MOS devices.

LDA STUDIES ON BUBBLE DYNAMICS OF SURFACTANT SOLUTION

Ronal Rai[1], Ajay Tripathi[1], Amitabha Bhattacharyya[1]

[1]*Department of Physics, Sikkim University, Gangtok, Sikkim, India.*

(Research Area: Soft Matter Physics)

Abstract: Surfactants are surface active agents which reduce the surface tension of a liquid.Surfactants consist of a hydrophilic head and hydrophobic tail, having an amphipathic structure. We have studied bubble motion and induced liquid motion due to rising bubble in a column filled with water and surfactant solutions of different concentration. In order to study such motion, Laser Doppler Anemometry, a contact free technique was used. Laser Doppler Anemometry is an optical contact free method for determining the flow rate of liquid or air by measuring the velocity of small particles added in that flow. When the particle passes through the measuring volume of the LDA system, it scatters light whose frequency is shifted on account of Doppler Effect. This frequency shift is used to calculate the particle velocity and therefore instantaneous liquid velocity.

Aqueous solutions of Sodium Dodecyl Sulfate (SDS) were studied. Bubble diameter and velocity decreases with the surfactant concentration and becomes constant after Critical Micellar Concentration (CMC). The liquid showed a strong horizontal motion on the bubble front compared to the rear end.In the surfactant concentration range studied, liquid motion is much smaller than in pure water. The presence of Critical Aggregation Concentration (CAC) can also be detected by these studies. The concentration region between CAC and CMC gives many interesting properties.

STUDY OF THE LEAD (II) REMOVAL FROM AQUEOUS SYSTEM BY MANGANESE OXIDE NANOPARTICLES

Rumman Zaidi[1], Saif Ullah Khan[2], I. H. Farooqi[2] and Ameer Azam[1]

[1] *Department of Applied Physics, Z.H. College of Engineering and Technology, Aligarh Muslim University, Aligarh, India*

[2] *Department of Civil Engineering, Z.H. College of Engineering and Technology, Aligarh Muslim University, Aligarh, India*

(Research Area: Nano and Biomaterials and applications)

Abstract: Here we report the synthesis of manganese oxide nanoparticles by simple co-precipitation method and its effectiveness in the removal of Pb(II) from aqueous solution. The prepared nanoparticles were characterized by X-ray diffraction studies (XRD) and Fourier-transform infrared spectroscopy (FTIR) to evaluate the structure of the material. The average crystallite size calculated by Debye-Scherrer equation was found to be 2.9 nm. Removal of lead was evaluated by using parameters such as time of equilibrium, initial pH, initial dosage of nanoparticles and concentrationof Pb(II). The results showed removal of lead was favored at an optimum pH of 4.Freundlich isotherm model was found to be a better fit for the obtained experimental data. The maximum removal capacity was found to be 85.0 mg/g. The removal kinetics followed the pseudo-second order model.

ELUCIDATION OF MORPHOLOGICAL, STRUCTURAL, SPECTRAL AND ELECTRONIC PROPERTY OF POLY THIOPHENE FILM FORMED OVER AIR-LIQUID INTERFACE

Subhajit Jana[1] and Rajiv Prakash[1]

[1]*School of Materials Science and Technology, Banaras Hindu University, Varanasi, Uttar Pradesh, India*

(Research Area: Polymers and Composite Materials)

Abstract: Performance and operational lifetime of organic material based electronic and optoelectronic devices depend on the degree of electron delocalization and its stability. Apart from material properties, another challenge in exploiting the potential of organic electronics is its cost, user-friendly, and ordered/crystalline thin film fabrication techniques. Therefore, a facile deposition technique is highly desired to have precise control over polymer chain ordering along with large area homogeneous thin film fabrication. In this work, the floating-film transfer method (FTM) has been utilized, which provides a large area, highly oriented, crystalline, and smooth polymer thin films.Chloroform solution ofpolythiophene and its derivatives were allowed to spread spontaneously over the liquid mixture of Ethylene glycol and Glycerol. The thin film was then transferred to a desired substrate and dried at 70°C for 2 hours in vacuum and characterized. The meridional XRD scan of the thin films show progressive diffraction (h00) peaks corresponding to side-chain interdigitation. Probing surface tension gradient driven flow, we extend the average coherence length (i.e., average crystal size) along (h00) direction up to nearly 14.56 nm, 15.80 nm and 25.26 nm for P3HT, PQT-12 and PBTTT respectively.As grain boundary resists charge

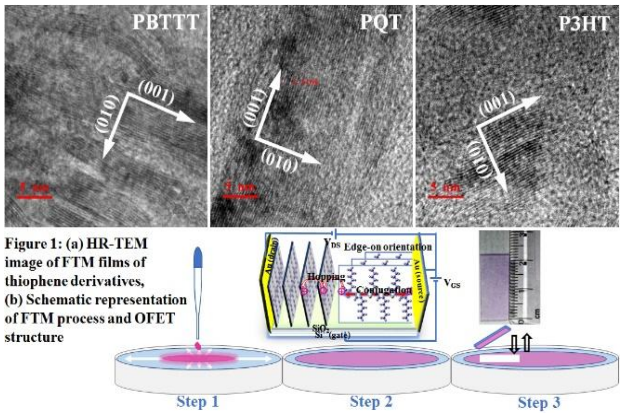


Figure 1: (a) HR-TEM image of FTM films of thiophene derivatives, (b) Schematic representation of FTM process and OFET structure

mobility, large coherence length justifies higher charge career mobility for PBTTT in comparison to other two polymers. Thus, FTM manipulates the relative orientation and spacing between molecules and enhances the electronic and optoelectronic functionality by assembling polymers at the air-liquid interface.

GREEN SYNTHESIS OF STRONG LUMINESCENT Si NPS USING ACTINIDIA DELICIOSA (AD)

Sweta Gurung[1] and Archana Tiwari[1]

[1]*Department of Physics, Sikkim University, Gangtok, Sikkim, India.*

(Research Area: Nano and Biomaterials & Applications)

Abstract: Water dispersible blue luminescent Si/SiO_2 Nanoparticles (NPs) were synthesized at room temperature by one step reduction of Si precursor APTES ((3-Aminopropyl)triethoxysilane) using *Actinidia deliciosa* as green reducing agent having an average size of 12.8±0.2 nm. HRTEM and SAED analysis show the presence of different sets of Si/SiO_2 planes and partial oxidation of the synthesized NPs. The absorption edge considering direct band gap transition is found to 3.34 eV which is usually due to the occurrence of absorption from crystalline Si core. The surface oxidation/defect is attributed to the red shift in the peak position in photoluminescence spectra. The stokes shift is found to be (~0.63 eV) which is particularly due to surface defect which is the result of surface oxidation. The PL quantum yield (PLQY) of as-prepared NPs are found to be highest (53%) on day 5 which is clearly due to synthesis of smallest size of NPs. This green synthetic route is low cost effective and does not require harsh conditions. AD has been used as a reducing agent for the first time in the synthesis of Si/SiO_2 NPs. The high QY of the as-synthesized NPs have numerous applications such as in biomedicine, bioimaging, neuroscience, solar cells etc.

THEORETICAL PREDICTION OF THE ELECTRONIC AND MECHANICAL PROPERTIES OF (6,1) CARBON NANOTUBE FROM LCAO-DFT APPROACH

Y Thakur Singh[a,b], D. P. Rai[b] and P. K. Patra[a]

[a]*Department of Physics, North-Eastern Hill University, Shillong, India*

[b]*Physical Sciences Research Center, Department of physics, Pachhunga University College, Aizawl, India*

(Research Area: Theoretical Condensed Matter Physics)

Abstract: Herein, we have studied the electronic and mechanical propertises of (6,1) single wall CNT (SWCNT) from Density Functional Theory (DFT). We report the comperative study of the electronic properties of (6,1) SWCNT with different bond length from GGA and DFT-1/2. CNTs are derived from the index number (n, m), lattice vectors and the orientation of the rolled graphene sheet. (6,1) SWCNT is a small band gap semiconductor. In both GGA and DFT-1/2 the band gap increases with increase in bond length with minimum formation energy at bond length 1.45 (arms). For mechanical properties we calculate Young's modulus for (6,1) SWCNT with bond lenth 1.45 (arms) from vibration technique using molecular dynamic simulations of the SWCNT. From our calculation we report the Young's moudulus value as 1.554 TPa.

References

[1] Gharbavi K, Badehian H, 2014 Comput. Mater. Sci. 82, 159-164.

[2] Gharbavi K, Badehian H, 2015 AIP Advances 5, 077155.

[3] M.S.M.Al-Khasrusi, K.Alzebdeh, T.Pelvez, 2016 Journal of Nanometerial 13-24.

SELF-ASSEMBLY OF ARSENIC NANOPARTICLES INTO MAGNETIC NANOTUBULES AND THEIR SERS ACTIVITY.

Laden Sherpa[1] and Archana Tiwari[1]

[1]*Department of Physics, Sikkim University, Gangtok, Sikkim, India.*

Abstract: Arsenic compounds in bulk as well as nanoscale, have been refined chemicallyand physically over the years to treat various diseases including cancer and tumors. Nano- arsenic such as single-layer of grey arsenic, arsenene, andits quantum dots have also been examined as novel class of materials with interesting optical and electronic properties. In comparison to othermetals, only limited works have been done on nano-arsenic and its derivatives. Nano-arsenic are synthesized using Bergenia cilliata roots extracts.The synthesised assemblies exhibit long range magnetic interactions and offer band-gapssimilar to that of arsenene.The synthesized As nanoparticles, with an average diameter of 13(1) nm, self-assemble into nanotubles with average Feret diameter of 530(20) nm. These As nanotubules/nanoparticles have direct band-gap of 2.737 eV and incorporate multiple defect related states within thegap. The presence of weak ferromagnetism in these nanotubules/nanoparticlesis attributed to the dipolar interactions amongst the charges on the defectsites. Owing to van der Waals interactions between nanotubules and smallernanoparticles, nanotubules present surface roughness and are utilized as surface enhanced Raman spectroscopy substrate for probing methylene blue dyewith anchemical enhancement of 10^3.

Unlike other works where an a contaminated systems such as arsenic contamination in water sources is dealt by introducing external magnetic NP as adsorber of the contaminant during the magnetic separation processes, here we present conversion of existing As ions in water into magnetic As NP/NT which can be separated from water by means of nano-filtration as well as by application of magnetic field.

INCREASE OF MAGNETIC PARAMETERS IN ZnO:Nd:Co Co-DOPED NANOPARTICLES

PREPARED BY SOL GEL METHOD

R. Chandramohan[1,2], Albert Manoharan[1], S. Valanarasu[3] and SR. Srikumar[4]

[1]*PG and Research Department of Physics, Sree Sevugan Annamalai College, Devakottai 630303, Tamilnadu, India*

[2]*PG Department of Physics, Vidhyaa Giri College of Arts and Science, Puduvayal-630108,Tamilnadu, India*

[3]*PG and Research Department of Physics, Arul Anandar College, Karumathur, Madurai -625514, Tamilnadu, India*

[4]*Department of Physics, Kalasalingam Academy of Research and Education, Krishnankoil- 626126,Tamilnadu, India.*

(Research Area: Condensed Matter Physics)

Abstract: Nanometer sized metal oxides and semiconductor materials are playing important role for the fabrication of next generation electronic circuits, magnetic and optoelectronic devices. Several metal oxide materials have been reported to reveal the ferromagnetic behavior at room temperature, however the beginning of ferromagnetism is not fully understood because some of the intrinsic defects are produced in the dilute magnetic metal oxide materials during the synthesis process. Zinc Oxide (ZnO) materials have wide range applications such as UV detectors, photo-catalysts, LED device, gas sensing behavior, spintronics applications, etc. The ZnO properties mainly depend on the intrinsic impurities and defects. We can reduce the defects of ZnO lattice by the inclusion of various doping elements like transition metal ions (Mn, Co, Fe) and rare earth metals (Nd, Gd, La). Because, the inclusion of rare earth (4f) and transition metal (3d) materials into the ZnO lattice can supply a possible approach to establish the energy levels in the band gap variation. In this study, ZnO nanoarticles were synthesized using *zinc*acetate dehydrate (Zn $(CH_3COO)_2$. $2H_2O$) and citric acid ($C_6H_8O_7$) using a sol gel process. Undoped (b) Co doped (c) Nd and Co co-doped ZnO nanoparticles were prepared under various dopant concentrations.The structural, optical, morphological electrical and magnetic properties were

studied and reported. The studies revealed the formation of hexagonal phase of the ZnO. Pristine, Co doped and Nd co-doped Co:ZnO nanostructures were successfully prepared using sol-gel combustion route. The XRD spectra confirmed the formation of single phase ZnO nanoparticles. There was no Nd and Co related impurity phases were observed in XRD spectrum. It was confirmed that Co and Nd elements were exactly included into the ZnO lattice. The lattice parameters were decreased slightly when the doped material Co and co-doped material Nd were added with ZnO. From the optical study, a reduction of band gap after doping is observed. The PL intensity studies support the XRD results that the crystallite size decreased with the inclusion of Co and Nd elements. The doping retained the phase with minor modification in the crystallite size. The morphology revealed agglomerated grains. The grain sizes varied. The increase in conductivity and ferromagnetism were observed due to doping while the undoped nanoparticles were non-magnetic. The co doping of 3% Ni and 3% Co produced the increased remenance and magnetic properties. The results are explained.

When Cobalt (Co) is doped into ZnO, ferromagnetic ordering starts to take place at room temperature and this could be explained based on a hopping mechanism of Co ions. Magnetic moment obviously rises with the addition of transition metal element, which assigned the ferromagnetic properties to Co-doped ZnO nanostructures and to the coexistence of Co^{2+} and Zn^{2+} ions through the double exchange mechanism. The observed ferromagnetism has also been explained based on exchange and super exchange interaction in Zn–O–Zn bond. The cobalt and neodymium doping in ZnO nonmaterial can enhance the magnetic properties and it can be used for spintronic applications.

A STUDY ON THE EFFECTS OF ETCHANT CONCENTRATION VARIATION ON CHEMICAL ETCHING CHARACTERISTICS OF 11.56 MeV/u $^{58}Ni^{14+}$ IRRADIATED MAKROFOL-E DETECTOR

Dipangkar Kalita[1], Raju Kalita[1],Yubaraj Sharma[2]and Atul Saxena[1]

[1]*Department of Physics, North-Eastern Hill University, Shillong, India*
[2]*Department of Physics, Don Bosco College, Tura, India*

(Research Area: Particle and Nuclear physics)

Abstract: Solid state nuclear track detector (SSNTDs) areamong the powerful tools in the study and application of nuclear radiations. It has numerous applications in nuclear physics, space research, anthropology, biomedical research, environmental science, particle identification, etc. It is well documented, that apart from the ion-detector characteristics, the development of the etched nuclear track depends on the chemical nature of the etchant, its concentration, and the temperature of chemical etchant. The bulk etch rate (V_G) and the track etch rate (V_T) are fundamental parameters that determine the shape of the etched track, which in turn gives the useful information about the detector and track-forming ion. V_G is determined directly from the rate of increment in the diameter of the nuclear track and by L_e-D (track length-diameter) method.In the present work, we study Makrofol-E detector exposed to a well-collimated beam of $^{58}Ni^{14+}$ ion of energy 11.56MeV/uat 45° angle with a fluence of 1×10^5 ion/cm^{2}at UNILAC, GSI, Darmstadt(Germany). The irradiated samplesare etched at four different normalities of the etchant NaOH viz. 2N, 3N, 4N, and 5N at the constant etching temperature of 60±0.5℃ and successive measurement of track diameter and track length are measured at different intervals of etching time, using a camera fitted transmitted light trinocular microscope and tracks are recorded. An optimum accuracy at different magnifications of the microscope have been usedviz. 10X objective magnifications (total magnification =150X) for track length and 40X objective magnification (total magnification = 600X) for track diameter measurements.

The results are tabulated and graphs of relevant pairs of variables plotted to visually depict their trend. As expected, both the etch rates V_G and V_T increases with increase in etchant concentration, but the rate of increase are disproportional as evidenced by the observed trend of the sensitivity of the SSNTD (defined as ratio of V_T and V_G) with etchant concentration. The implication of the result is discussed.

ACHIEVING LONG-TERM AMBIENT AIR-STABILITY IN CUBIC $CsPbBr_3$ PEROVSKITE QUANTUM DOTS USING THREE PRECURSOR METHOD

Surakcha Thapa, Karishma Bhardwaj, Siddhant Basel,SajanPradhan, Charlotte J. Eling Ali M. Adawi, Jean-Sebastien G. Bouillard, Graeme J. Stasiuk, Peter Reiss, Anand Pariyar and Sudarsan Tamang

Department of Chemistry, Sikkim University, Gangtok, Sikkim, India.

(Research Area: Nano and Biomaterials & Applications)

Abstract: Colloidal nanocrystals of caesium lead halide perovskite ($CsPbX_3$, X= Cl, Br, or I)are highly studied materials in the field of photovoltaics , optoelectronics, LEDs owing to their high photoluminescence (PL) quantum yield (QY), narrow emission line width, high defect tolerance, size and shape tunable band gaps covering most of the visible region. One of the major drawbacks, however, is their structural instability. Consequently, phase stability issue must be addressed in order to achieve practical application with these materials. Among all the phases of $CsPbX_3$ (X = I or Br)their cubic phase is the most unstable at room temperature under ambient conditions. In this talk, we will address how tuning surface chemistry can lead to improved stability. We discuss improved phase stability of cubic$CsPbX_3$ (X = I or Br)quantum dotsin ambient airobtained by using molecular halogen as halide precursor. The talk will also focus on underlining mechanism of surface passivation and unprecedented stability

EFFECT OF PRECURSOR CONCENTRATION ON STRUCTURAL AND GAS SENSING PROPERTIES OF NANOSTRUCTURED V_2O_5 THIN FILMS

Ravinder Gandasiri[1], C.J. Sreelatha[1]

[1]*Materials Research Laboratory, Department of Physics, Kakatiya University, Warangal, Telangana, India.*

(Research Area: Thin Films)

Abstract: Vanadium pentoxide(V_2O_5) thin films wereprepared by the spray pyrolysis techniqueon cleaned glass substrates at thedeposition temperature of 325°C. The XRD patterns revealedthat the crystallinity of the V_2O_5filmswasincreased with the increase ofprecursor concentration. SEM analysis illustrated that the well-defined nanostructuredmorphologywas observed at 0.075M. The crystal size of the thinfilms varies from 12nm to 25 nm, with the increase of concentration of the precursor solution.XPS analysis confirms the presence of V^{5+} oxidation state of vanadium in V_2O_5 film. The sensing properties of V_2O_5 films towards acetone, methanol, toluene and xylene vapours were observed. V_2O_5 thin filmdeposited at the concentration of 0.075M, shown high response and recovery times towards 100ppm of toluene gas. The effect of precursor (ammonium vanadate) concentration on structural and gas sensing properties of the films have been investigated and discussed.

Keywords: Spray pyrolysis, V_2O_5, concentration, gas sensingand toluene.

MATHEMATICAL MODELS IN FRACTAL ANTENNA DESIGN: A REVIEW

Leeladhar Chouhan[1]

Department of Physics, Kokrajhar Govt. College, Kokrajhar, Assam, India-783370

(Research Area: Mathematical Modeling)

Abstract: Recently, telecommunication systems have been emphasizing on miniaturization, high efficiency and low cost. Thus antenna minimization has become a wide field of research. In antenna design, fractal geometries have attracted widespread attention becauseminiaturization process can be achieved through theimplementation of self scaling, space filling and selfsimilarity properties of fractals.The term "fractal" was coined in 1975which means non-regular andnever ending pattern. Fractals in fact have fractional dimensionsand they have been applied in diverse fields as geology, medicine, cosmology, engineering, computer graphics and animation, and social sciences.Antennas based on fractals have significantly improved antenna features such as smaller size, operating in multi-frequency bands, with improved power gain and efficiency. This paper discusses the mathematical models of common fractal antenna like Sierpinski gasket model,Minkowski fractal model, Koch curve model and Hilbert curve model.

Keywords: Fractal geometries, Sierpinski gasket, Koch Curve, Hilbert Curve

PRECURSOR FLOW IN ONE-SHOT TWO DIMENSIONAL FORCED FOAM DRAINAGE IN NATURAL SURFACTANT SYSTEM

Ambika Pradhan[1] and Amitabha Bhattacharyya[2]

[1]*SRM University, Sikkim, Gangtok 737102 Sikkim. India.*

[2]*Department of Physics, Sikkim University, Gangtok, Sikkim, India.*

Abstract: Surfactant monolayer absorbed at air/water interface stabilizes the foam. An important factor deciding the stability of foam is drainage, which is the flow of intervening liquid in foam as a result of gravity, surface tension and viscosity. Drainage plays a vital role in brewing, metallurgy and petroleum industries. We report, for the first time, one shot two dimensional forced foam drainage in a natural surfactant extracted from *Sapindus mukorossi(Ritha).* The draining wave-front flows vertically due to gravityand spreads horizontally due to capillarity as it descends. The vertical front position proceeds with time in a power law whose exponent indicates a Poiseuille type flow, like synthetic surfactants. The drainage wave-front reveal a conic form downstream producing an expanding ellipsoid with time. The intensity of light at any point (gray scale) is taken as an indication of liquid fraction. The liquid fraction profile indicates the beginning of propagation of the drainage wave-front, its initial build-up at the top of the foam and finally the flow downstream. Liquid fraction analyses follow a normal Gaussian distribution along the horizontal direction. There is an asymmetric Gaussian distribution along the vertical which distorts after 10 seconds, indicating two types of flow occurring simultaneously through the foam. These two movements have not been previously reported in the literature for synthetic surfactants. Further studied are required to understand these movements through the foam.

Keywords: Forced Drainage, Natural surfactant, Foam Stability, Aqueous Foam, Liquid Fraction Profile

Electrical conductivity studies on lithium sulfate doped molybdenum phosphateglasses

N. Sivasankara Reddy[1]

[1]*Department of Physics, School of Engineering, Presidency University, Bangalore, India*.

(Research Area: Energy Materials)

Abstract: Lithium ion conducting glasses have attracted considerable importance because of their possible applications in solid state batteries and electrochemical devices. In this work we report Li^+ ion transport properties of xLi_2SO_4-$30Li_2O$-$(70-x)[0.70P_2O_5:0.30MoO_3]$ (x=5, 10, 15, 20 and 25 mol%) glasses. Glasses are fabricated using melt quenching technique and their amorphous nature is confirmed by XRD studies. Conductivity measurements are carried out in the frequency range of 100 Hz - 11 MHz over and a temperature range of 313 K to 463 K. Impedance plots exhibit good semicircles and reveals the domination of ionic conductivity. D.C conductivities (σ_{dc}) extracted from impedance plots follow Arrhenius behavior and d.c activation energies (E_{dc}) are estimated from regression analysis. Activation energies (E_{dc}) decreases and d.c conductivities (σ_{dc}) increases with the addition of Li_2SO_4 content. The impedance and modulus spectroscopic plots (Z″ and M″ versus frequency) reveals that the relaxation mechanism of Li^+ ions in the investigated glasses is due to localized movement of charge carriers (short range), temperature dependent and of non-Debye type.

Keywords: Ion conductivity, activation energies, impedance spectroscopy, relaxation

SYNTHESIS AND CHARACTERIZATION OF Ca and Zr MODIFIED $BaTiO_3$ FERROELECTRIC CERAMICS

M.A. Bilya, M.U. Sarki, A.A. Mundi, M.M. Mustapha

Nasarawa State University, Keffi, Faculty of Natural and Applied Sciences, Department of Physics, Nasarawa State, Nigeria.

(Research Area: Energy Materials)

Abstract: A lot of synthesis methods have been developed for the preparation of barium titanate powders. But the successful synthesis of BaTiO3 nanopowders with unique dielectric properties largely depends on the purity and microstructural features (Ashiri, et al., 2011). Thus, in this research, Ca and Zr modified $BaTiO_3$ ferroelectric ceramics ($Ba_{1-x}Ca_xZr_{0.05}Ti_{0.95}O_3$: x = 0.00, 0.03, 0.06, 0.09, and 0.12) was Synthesized and characterized, via the solid state synthesis technique. The structural and microstructural analysis was carried out using XRD for improved single phase at different temperatures. The dielectric constant, ε of the material was measured as a function of temperature. It has been observed that as the grain size decreased, the maximum dielectric constant (ε_{max}) decreased, but the transition temperature increased (Rawat et al., 2015). high dielectric constant, relatively low dielectric losses, large voltage tunability of the dielectric constant, as well as a good chemical stability was recorded.

Keywords: Ferroelectric, Characterize, Nanopowder, Dielectric, Transition temperature.

References

[1] Ahmadu, U., Muazu, A., and Umar, S.(2018). Physical Properties of Porous Pure and Zr/Sn-Doped Nanocrystalline BaTiO3 Ceramics. Recent Advances in Porous Ceramics. Intech Open.Chpt.9, Pp. 147-170.http://dx.doi.org/10.5772/intechopen.75500

[2] Gattu, S., Prasadu, V.D., and Ramesh, K.V., (2015). Effect of Zr on Structural and Dielectrical Properties of (Ba0.9Mg1.0)(ZrxTi1−x)O_3 Ceramics. Advances in Materials Physics and Chemistry. 5, 419. http://dx.doi.org/10.4236/ampc.2015.510042.

[3] Islam, S., Siddika, A., Khatun, N., and Hossain, M.S., (2018). Structural, Dielectric and Electric Properties of Manganese-Doped Barium Titanate. International Journal of Nanoelectronics and Materials. Malaysia. *Volume 11, No. 4, Pp.* 419 – 426.

[4] Kumar, G.S., Mazumder, R., Pratihar, S.K., (2015). Department of Ceramic Engineering National Institute of Technology Rourkela–769008, Odisha, India. Pp. i-ii.

[5] Panirahi, N.R. (2010).On the Structure and Dielectric Study of Iso- and Alio-Valent Modified BaTiO3 Ceramics.Department of Physics National Institute of Technology Rourkela 769 008, India. A P.hD. Project.

[6] Rawat, M, Chawla, M., Rawat S., and Fahim, M., (2015). Synthesis and Characterization of Sol-Gel Derived Barium Calcium Zirconate Titanate Ba0.8Ca0.2)(Zr0.2Ti0.8)O3 Powder and Ceramics. International Global Journal for Research Analysis.Volume4, Issue , ISSN No 2277-8160 Pp. 1-4.

PRESSURE DEPENDENT STRUCTURAL PHASE TRANSITION STUDIES ON $BiFeO_3$ DOPED $PbTiO_3$SOLID SOLUTION SYSTEM

Pragya Singh, Chandan Upadhyay and Dhananjai Pandey

School of Materials Science and Technology, Indian Institute of Technology (BHU), Varanasi, India.

(Research Area: Organic and Inorganic Materials)

Abstract: Pressure is a clean thermodynamic variable which induces a rich variety of structural phase transitions. Among the various functional materials, $PbTiO_3$ is a model compound whose high pressure behavior has been revisited extensively because of its technological importance for the piezoelectric industry[1]. However, its structural phase transition sequence at high pressures has been found to be quite controversial. One of the many pictures presented reports that pressure can induce polarization rotation in simple tetragonal ferroelectrics just likeobserved across the morphotropic phase boundary of commercially important piezoelectric solid solution systems[2]. Another picture claims that pressure induces antiferrodistortive type structural transitions in pure $PbTiO_3$followed by emergence of a reentrant ferroelectric phase[3]. We have attempted to address these controversies by performing a high pressure structural study on a tetragonal composition of 50% $BiFeO_3$-doped$PbTiO_3$solid solution system using synchrotron x-ray diffraction measurements. We have found that at quite moderate values of pressure (~2 GPa), the tetragonal P4mm phase of the system transforms to monoclinic Cc phase which permits rotation of ferroelectric polarization vector as well as oxygen octahedral tilting leading to antiferrodistortive type transition. On further increasing the pressure, the monoclinic distortions and the ferroelectric polarization start decreasing, but after a critical value of pressure (~7 GPa), they start increasing which hints towards another isostructural phase

transition. Oxygen octahedral tilting provides an efficient mechanism for accommodating volume reduction in this reentrant ferroelectric phase. The results obtained also provide an insight towards designing of new environmentally friendly Pb-free piezoelectric compositions.

Keywords: High pressure, morphotropic phase boundary, perovskites, functional materials.

References:

[1] Jaffe, B., Cook, W.R. and Jaffe, H., Piezoelectric Ceramics (Academic Press, New York, 1971).

[2] Wu, Z. and Cohen, R.E., 2005. Pressure-induced anomalous phase transitions and colossal enhancement of piezoelectricity in PbTiO3. Physical review letters, 95(3), p.037601; Ganesh, P. and Cohen, R.E., 2009. Pressure induced phase transitions in PbTiO3. Journal of Physics: Condensed Matter, 21(6), p.064225.

[3] Kornev, I.A., Bellaiche, L., Bouvier, P., Janolin, P.E., Dkhil, B. and Kreisel, J., 2005. Ferroelectricity of perovskites under pressure. Physical review letters, 95(19), p.196804; Kornev, I.A. and Bellaiche, L., 2007. The nature of ferroelectricity under pressure. Phase Transitions, 80(4-5), pp.385-413.

TUNABLE NON-HERMITIAN ACOUSTIC FILTER

Sandeep Puri[1]

[1]*Department of Physics and Astronomy, University of Texas Rio Grande Valley, Edinburg, TX 78539, USA*

(Research Area: Non-Hermitian Quantum Mechanics)

Abstract: We propose and design an acoustic super-lattice that acts as a tunable filter depending on the degree of non-Hermiticity. The super-lattice composed of two concatenated sub-lattices, one Hermitian and the other non-Hermitian. The degree of non-Hermiticity changes width and position of the gaps of the band structure of the non-Hermitian sub-lattice as well as the width and position of the resonances which provides a powerful knob to absorb or reflect several frequencies at will. Our proposed tunable acoustic filter can be extended to higher frequency ranges such as ultrasound and other areas like photonics.

Keywords: Tunable filter, non-Hermitian, super-lattice and sub-lattice.

MONTE CARLO STUDY OF PHASE TRANSITION IN MODIFIED LEBWOHL LASHER MODEL

Enakshi Guru[1]

[1]*Department of Physics, Rishi Bankim Chandra College, Naihati, 24 pargana, West Bengal, India.*

(Research Area: Soft Condensed Matter)

Abstract: Lebwohl lasher model is used for the system having lattice dimension three and it exhibits the nematic isotropic phase transition. The modified model discussed in this paper, consists of rod-like molecules placed at the sites of two dimensional lattice and spin of molecules are three dimensional. Hamiltonian of the system isH=-ijP2(cosij), is the angle between the spin of two nearest- neighbour. We study the histogram of energy and order parameter for 3 to 5 million cluster within 12 to 15 temperature near transition. Wolf algorithm is used with periodic boundary condition for lattice dimension 10 to 240. Specific Heat and susceptibility were calculated from the fluctuation of energy and it is plotted with respect to temperature near the transition. Critical temperature is obtained from peak position of specific heat, order parameter susceptibility, order parameter derivative and derivative of energy. The phase transition is continuous. Dimensionless critical temperature is 0.55 (from order parameter scaling) to 0.57 (from Cv scaling)

PREPARATION, CHARACTERIZATION OF BIOSYNTHESIZED ZnO BASED UV-SHIELDING MATERIAL

Abhijit Nath[1] andMrityunjoy Mahato[1]

Department of Basic Sciences and Social Sciences, School of Technology, North-Eastern Hill University, Shillong, India.

(Research Area: Nano and Biomaterials & Applications)

Abstract: ZnO is a semiconductor material with band gap energy 3.37 eV and binding energy 60 meV. [1] It is used as UV shielding material because it shows absorbance peak in the UV region. Its functional properties such as nontoxic, gas-sensors, photocatalyst, optical devices, made this important in the laboratory applications. In addition, ZnO is low cost material in comparison to other metal oxides [2]. But it cannot completely block the UV light. We have synthesized ZnO nanoparticles by using bio-synthesis method using extract of chayote (Sechium edule) fruit. The as prepared ZnO were taken to grow heterostructure of Bi_2O_3-ZnO by controlled microwave method. The prepared ZnO and its heterostructures were characterized by TEM, XRD and UV-vis spectroscopy. UV absorbance peak was found at 372 nm for ZnO and at 247 nm for Bi2O3. For heterostructure, the peak was at 225 nm and 370 nm. Our finding is, in EG solution, ZnO-Bi2O3 can block more 90% UV-radiation. Further it can be used for composite preparation to get transparent and flexible film.

Keyword: UV-shielding Material, ZnO, Heterostructure.

ELECTRICAL CONDUCTIVITY STUDY OF NANO-PHASED MATERIALS: FREQUENCY AND TEMPERATURE DEPENDENCY

Aditi Sengupta [a, b*], Amartya Acharya[a], Subhajit Roy[c] and Sanjib Bhattacharya[a]

[a] *Composite Materials Research Laboratory,Department of Engineering Sciences and Humanities, Siliguri Institute of Technology, Darjeeeling-734009, West Bengal, India*

[b]*Department of Electronics and Communication Engineering, Siliguri Institute of Technology, Darjeeeling, West Bengal, India*

[c]*Department of Electrical Engineering, Siliguri Institute of Technology, Darjeeeling, West Bengal, India*

(Research Area: Energy Materials)

Abstract: A glass-ceramic sample, $0.1Li_2O$-(0.9)(0.05ZnO-0.475MoO_3-0.475SeO_2) and it's crystalline counterpart have been prepared using melt quenching and slow cooling routes respectively. The study of XRD patterns reveals the dispersal of dissimilar types of nanocrsytallites in amorphous glassy matrices. The ionic conductivity as well as frequency and temperature dependent conductivity have been studied, which follows Jonscher's universal power-law and Almond-West formalism. The variation of activation energy corresponding to AC conductivity (E_{AC}) with composition has also been studied. The frequency independent conductivity (plateau region) in low-frequency zone is caused by sub diffusive motion of Li^+ ions. Moreover, in the high-frequency dispersive region, the conductivity arises because of correlated and pseudo-three-dimensional motion of Li^+ ions in percolating networks. The master curve in scaling analysis signifies temperature independency of conductivity relaxation process.

Keywords: Nano-phased materials; Glass-ceramics; Composite materials; X-ray diffraction; Ionic conductivity; Li^+ ion migration.

ELECTRONIC AND MAGNETIC PROPERTIES OF DOUBLE PEROVSKITESPb_2XOsO_6 (X=Co, Ni)

Bishnu Prasad Belbase[1,2], Shalika Ram Bhandari[1,2,3], Madhav Prasad Ghimire[1,2,3]

[1]*Central Department of Physics, Tribhuvan University, Kirtipur, 44613, Kathmandu, Nepal*

[2]*Condensed Matter Physics Research Center, Butwal-11, Rupandehi, Nepal*

[3]*Institute for Theoretical Solid State Physics, IFW Dresden, Helmholtzstr-20, 01069 Dresden, Germany*

(Research Area: Condensed Matter Physics)

Abstract: The electronic and magnetic properties of double perovskites Pb_2XOsO_6 (X=Co, Ni) have been studied by using density functional theory within generalized gradient approximation. By replacing Co from Pb_2CoOsO_6 (PCOO), Pb_2NiOsO_6 (PNOO) is formed. PCOO and PNOO are found to be A-type anti-ferromagnetic and ferrimagnetic metals respectively without the application of spin-orbit coupling (SOC). Density of state plot reveals that, in both materials there is a contribution from every atoms near the Fermi level and strong hybridization between Os-5d and O-2p. Since this system is highly correlated system, cooperative effect of SOC and coulomb correlation (U) have high chance of opening the gap in these materials. So, we first applied U in the system, which didn't open a gap but shows a significant changes in DOS indicating possibilities of opening a gap by cooperative effect of SOC and U.

Keywords: Double perovskites, Density functional theory, Coulomb correlation

COPPER NANOCLUSTERS: A NOVEL PHOTOLUMINESCENT PROBE FOR DETECTION OF 2,4,6-TRINITROPHENOL

Chandra Shekhar Pati Tripathi

Department of Physics, Institute of Science, Banaras Hindu University Varanasi,India.

(Research Area: Nano and Biomaterials & Applications)

Abstract: In the recent years, metal nanoclusters, which are composed of a few to roughly a hundred atoms have gained a great deal of interest in the fields of sensing, catalysis and imaging applications due to their excellent fluorescence, low toxicity, high quantum yield, good water-solubility and biocompatibility. Researchers have focused mostly on the synthesis, and characterization of gold and silver nanoclusters for a range of analytical application. However, very little attention has been paid to the fluorescent copper nanoclusters (CuNCs) [1-2].

In this work, we have developed a photoluminescence (PL) based selective and sensitive detection method for the detection of 2,4,6-trinitrophenol (TNP) by PL quenching and hydrogen peroxide by PL enhancement using bovine serum albumin stabilized copper nanoclusters (BSA-CuNCs). The highly stable, and water soluble blue emitting copper nanoclusters were prepared by a simple chemical reduction method using commercially available protein BSA. The quenching of PL of BSA-CuNCs were found highly selective and sensitive towards TNP. Under the optimized conditions, the PL intesnity of as synthesized BSA-CuNCs were observed to be decreasing linearly with increasing concentration of TNP in the range of 0-15 μM and the limit of detection was found to be 60 nM (3σ/k). The proposed sensor was also tested in natural water samples and was found to be rapid and highly selective and for the detection of TNP. The probe is also capable of sensing hydrogen peroxide. In the presence of hydrogen peroxide, the PL of

the BSA-CuNCs was found to be enhanced with increasing with concentration of H_2O_2. This shows the potential application of BSACuNCs as a multiresponsive photoluminescent sensor.

References:

[1] L. Shang, S. Dong, G.U.J.N.t. Nienhaus, Ultra-small fluorescent metal nanoclusters: synthesis and biological applications, 6 (2011) 401-418.

[2] X. Hu, T. Liu, Y. Zhuang, W. Wang, Y. Li, W. Fan, Y. Huang, Recent advances in the analytical applications of copper nanoclusters, TrAC Trends in Analytical Chemistry, 77 (2016) 66-75.

SPECTROSCOPIC ELLIPSOMETRY: A POWERFUL TOOL TO STUDY Si:H NANOCRYSTALS

Romyani Goswami

Department. of Physics, Surya Sen Mahavidyalaya, Surya Sen Colony, Siliguri, Darjeeling, West Bengal, India.

(Research Area: Solar Energy)

Abstract: Structural study on hydrogenated silicon thin film network is very essential for application of the films in solar cell technology and other optoelectronic devices. The third generation solar cells are basically based on nano-crystalline and nano-porous materials. The study of Si:H films deposited around the edge of crystallinity is being very promising nowadays because of the better structural order, device grade photosensitivity and lower light induced degradation of the edge materials compared to conventional amorphous Si films. A detailed study of Spectroscopic ellipsometry (SE) has been done to investigate the as deposited hydrogenated nanocrystalline silicon films (nc-Si:H) and the same films after thermal annealing. The nc-Si:H films have been deposited initially by radio frequency plasma enhanced chemical vapor deposition (RF PECVD) varying deposition power density from 0.03 W/cm2 to 0.46 W/cm2. Different bulk compositions of the as deposited (nanocrystalline) and annealed (polycrystalline) films have been calculated from the fitted parameters obtained from the simulation of the ellipsometry data by Bruggeman effective medium approximation (BEMA) method. It is observed in the as deposited films that they have more compact and void free structure in the bulk layer at low power deposition region. For the annealed films it is observed that the low power deposited films have higher crystallinity at the bulk layer with fewer voids but in the surface roughness layer void fraction dominates in all the low and high power

deposited films. The results obtained from SE measurement have been compared with Raman study and TEM of both of the as deposited and annealed films.

Keywords: nanocrystalline silicon, spectroscopic ellipsometry, transmission electron microscopy, Raman spectroscopy

BAND GAP ENGINEERING OF$Hg_xBe_{1-x}X$ (X= S, Se & Te)TERNARY ALLOYS - A THEORETICAL INITIATIVE USING DFT BASED FP-LAPW APPROACH

Manish Debbarma[a], Utpal Sarkar [a], Surya Chattopadhyaya [a]

Department of Physics, Tripura University, Suryamaninagar, Tripura, India

(Research Area: Soft Condensed Matter)

Abstract: Structural, electronic and optical features of mercury-beryllium-chalcogenide ternary alloys have been computed employing density functional theory (DFT) based FP-LAPW approach. Structural features have been computed with Wu-Cohen (WC)-GGA functional for each alloy system. The electronic properties are explored with GGA+U, modified Becke-Johnson (mBJ), Engel-Vosko (EV)-GGA functional and direct-indirect band gaps. Bang gap for each alloy system decreases nonlinearly with Hg-concentration. Chemical bonding between beryllium and chalcogen mercury and chalcogen are investigated. In case of optical transitions, the chalcogen-p of valence band as initial states and Be-3s, 2p as well as Hg-6s states of conduction band as final states play the dominant role.In each alloy system, nature of variation of each of the static dielectric constant and static refractive index are studied. Several calculated properties are found to agree well with the corresponding experimental findings.

MODIFICATION OF TRANSPORT PROPERTIES WITH GRAPHENE OXIDE REINFORCEMENT IN ZINC OXIDE THIN FILMS

Mrinmoy Chakraborty and Rabindra N. Gayen

Department of Physics, Presidency University, 86/1 College Street, Kolkata-700073

(Research Area: Semiconductor Thin Films)

Abstract: Graphene oxide(GO), a 2-D nanomaterial with unique electrical properties,is considered as one of the most promising materials which enhances the optoelectronic properties of zinc oxide(ZnO) by decreasing recombination and increasing lifetime of photo-generated charge carriers of host matrix.Here we report the fabrication of highly transparent ZnO-GO nanocomposite thin films by easy,low cost sol-gel spin coating technique and demonstrate the transport characteristics modification of ZnO with incorporation of little amount of GO sheets by temperature dependent complex impedance spectroscopy. Microstructural and optical studies confirm the formation of highly transparent composite thin films with nanocrystalline hexagonal ZnO and GO sheets. Temperature dependent impedance spectroscopic study in the frequency range 100 Hz-5 MHz reveals the electrical responses from grain,grain boundary and interfaces. The Nyquist plot is fitted by suitable electrical circuit model comprised of several parallel RC circuits in series and distribution of relaxation times(τ = RC) is estimated which are arising out of different electrical responses from grains,grain boundaries and interfaces under the application of small ac signal.Temperature variation of relaxation times confirmed the grain boundary effect on charge transport in the thin films. Also the significant decrease of τ value attributed to grain-boundary contribution in the GO reinforced ZnO thin film confirms that little amount of conducting GO network modify the grain-boundary of pristine ZnO and facilitates better charge transport through it. Temperature variation of frequency dependent dielectric constant, loss

factor and ac conductivity is also studied for the ZnO-GO nanocomposite thin film, a suitable material for transparent optoelectronic devices.

Keywords: Sol-gel; Graphene oxide; Nanocomposites; Impedance spectroscopy

ENHANCEMENT OF PROPERTIES BY MEANS OF FORMULATION OF BINARY MIXTURE OF TWO ANTIFERROELECTRIC LIQUID CRYSTALS

Kartick Ch. Dey

Department of Physics, Acharya Prafulla Chandra Roy Government College, Siliguri, West Bengal, India

(Research Area: Soft condensed matter)

Abstract: To observe how the properties are influenced, two antiferroelectric liquid crystals [$C_3F_7.CH_2O.C_6H_{12}.O.Ph.COO.Ph.Ph.COO.CH^*(CH_3)C_6H_{13}$] and [$C_3F_7.CH_2O.C_6H_{12}.O.Ph(F_2).COO.Ph.Ph.COO.CH^*(CH_3)C_6H_{13}$] are mixed in varying wt.%. It has been found that the melting point of the mixtures when plotted against wt.% of any one compound exhibits a arc shape with lowest dip at mid wt.%. For a mixture of 50wt.% of each, the melting point is drastically decreased to 39.8^oC compared to those of pure compounds [61.0^oC and 63.2^oC], indicating the formation of eutectic binary mixture. The binary eutectic mixture shows the same phase sequence as that of pure compounds [Cr–SmC_A*–SmC*–SmA*–Iso] but with increased range of SmC_A* phase [46.2^oC] compared to pure compounds [33.0^oC, 22.0^oC]. The critical field for suppression of GM is observed to increase which indicates helical structure in the mixture is more stable. Spontaneous polarization maintains almost in the same range [221.7 nC/cm^2] as that of the pure compounds[210.0 nC/cm^2 and 191.7nC/cm^2] which is moderate one and suitable for display application. The eutectic binary mixture maintains the switching time in a few hundred microseconds range[650 µs] as like pure compounds [340µs, 500 µs], which is also suitable for display applications. The activation energy is observed to decrease [30.25 kJ/mol] compared to the pure compounds [38.19 kJ/mol and 44.34 kJ/mol] which indicates less driving force is required for the relaxation to initiate.

Keywords: eutectic binary mixture; critical field; spontaneous polarization; switching time; activation energy.

HALF-METALLICITY IN EQUIATOMIC QUATERNARY HEUSLER ALLOY PtFeCrAl: A FIRST PRINCIPLE STUDY

Kunal Labar[1,2], Amit Shankar[2] and Ranjan Sharma[1]

[1]*Deptartment of Physics, Cooch Behar Panchanan Barma University, Cooch Behar, West Bengal, India.*

[2]*Condensed Matter Theory Research Lab, Department of Physics, Kurseong College, Kurseong, Darjeeling, India.*

(Research Area: Energy Materials)

Abstract: The first principle method has been implemented in determining the half-metallicity of a new class of equiatomic quaternary Heusler PtFeCrAl and its befitting possibility in the spintronic applications. The structural optimization leaves the material stabilized in LiMgPdSn type structure of *F-43m* space group with lattice constant of 5.97 Å. The analysis of the formation energy and the dynamical stability further supports the possibility of synthesis in laboratory for further study. The studied material is 100 % spin-polarized near the Fermi energy level, with a half metallic gap of 0.03 eV in the minority spin channel and a metallic type for the majority spin channel. The magnetic profile of the material shows its ferromagnetic nature with a magnetic moment of 3.00 μ_B per formula unit which is in compliance with the Slater Pauling rule of $M_T = Z_T - 24$. In overall, the 100% spin-polarized half-metallic ferromagnetic nature of this material is predicted that may be suitable for effective spintronic applications.

OPTICAL PROPERTIES OF LIQUID CRYSTAL NANOCOMPOSITE

Pawan Singh, Narinder Kumar, Khem B. Thapa and Devesh Kumar

Department of Physics, School of Physical and Decision Sciences, Babasaheb Bhimrao Ambedkar University, VidyaVihar, Rae Bareli Road, Lucknow (U.P.) India.

(Research Area: Liquid Crystals and Solar Cell)

Abstract: In this work, we have calculated the optical properties of liquid crystal nanocomposite with inclusion of silver nanoparticles. Such system also supports the Dyakonov surface waves, which propagates at the interface of isotropic and nanocomposite. The different size of nanoparticles in media can tune the surface waves and optical properties of whole nanocomposite. We have calculated the dielectric constant of LC nanocomposite for two different orientations of LC molecules. The LC nanocomposite also shows the some negative refractive index for certain size and filling fraction of nanoparticles that are supported with surfaces waves in nanocomposite. To understand the physics of the LC nanocomposite with inclusion of silver nanoparticles, we have studied the optical properties of NC calculated using transfer matrix method (TMM) at different orientation of LC molecules.

Keywords: Dyakonov surface wave, nanocomposite, silver nanoparticle, TMM

References

[1] T. Matsui, Appl. Phys. Exp., **08**, 072601, (2015).

[2] M. I. Dyakonov, Sov. Phys. JETP, **67**, 714, (1988).

[3] O. Takayama et al., Electromagnetics, **28,** 126, (1988).

[4] E. E. Narimanov, Phys. Rev. A, **98**, 013818, (2018).

STUDY OF DEPENDENCY OF INITIAL CONDITIONS AND TEMPERATURE DURING GROWTH OF TIN OXIDE ON Ag(111)

Suvankar Chakraborty[1], Krishnakumar S R Menon[2]

[1]*Department of Applied Sciences, Haldia Institute of Technology, Haldia Purba Medinipur, 721657, West Bengal, India*
[2] *Surface Physics and Material Science Division, Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Kolkata 700064, India*

(Research Area: Thin Films)

Abstract: Tostudy the dependency of the growth on initial conditions and temperature, tin oxide

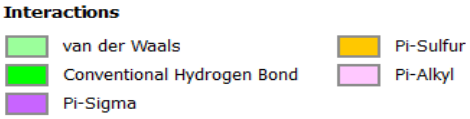
was grown starting from Sn/Ag(111) alloy. Sn was deposited on Ag(111) at 473 K for 3 ML coverage which is a moderate thickness to start with. The grown films were studied at room temperature by a combination of low energy electron diffraction (LEED) and angle resolved photoemission spectroscopy (ARPES). Deposited Sn forms bulk alloy with Ag(111) as noticed from the LEED pattern. the alloy sample was annealed at 523 K in oxygen environment keeping the same oxygen pressure used for growing tin oxide for 15 minutes. LEED pattern confirms that the Sn alloy is not fully oxidized and still signature of metal alloy was shown. Next, the same sample was annealed at 573 K 15 minutes which was the growth temperature of tin oxide, keeping all other parameters fixed. The LEED pattern transform into exactly the same pattern as was observed for tin oxide during to co-deposition. So it is clear from the LEED study that same final phase would be formed for tin oxide, irrespective of the starting condition. Even though the LEED patterns appear to be the same, the details of the electronic structure obtained from the ARPES measurements appears to be marginally different

depending on the route of the oxidation process. So, co-deposition of Sn metal in oxygen environment on metal substrate for growth of tin oxide eventually gives the surface structurally the same tin oxide formed by oxidizing Sn/Ag alloy, but the electronic structure is not same clearly indicating the role of oxidization is important.

IN-SILICO ANTI-CANCER STUDIES ON PHYTOCHEMICAL, COUMESTROL

P. Vinduja, P. Muraleedharan, Chandana, K.

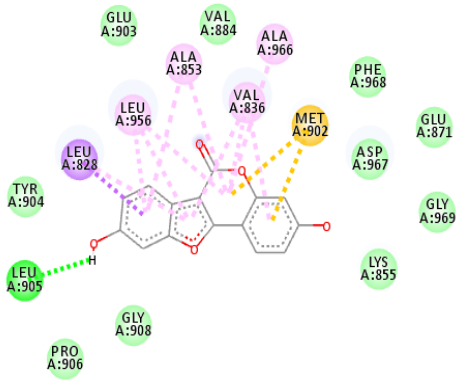
Department of Chemistry, University of Calicut, Calicut -673635, India



(Research Area: Mathematical Modeling)

Abstract: Cancer disease is defined as the uncontrolled multiplication of abnormal cells. Natural product based computational studies are very popular in this area and it is an excellent technique to find novel biological remedies for a variety of diseases including cancer.Coumestrol is a phytoestrogen found in soya bean products and is considered a possible therapeutic agent against various types of cancers.Kinase target proteins such asB-RAF, JAK3, and MEK1 are the reasons for multiple human cancers and therefore they can be regarded as promising cancer therapy targets.

Molecular docking is an excellent way to study protein-ligand interactions, as they play a crucial role in drug design.Hence molecular docking investigation was carried out to study the interaction of coumestrol with the proteins such as B-RAF, JAK3, and MEK1, which revealed the high inhibition activity of coumestrol on various types of cancer-causing proteins. We found that the compound shows good interaction with all the three targets, the binding energy values being -9.5, -9.3, and -9.1 kcal/mol respectively with JAK3, B-RAF, and MEK1. More interestingly, this binding affinity of coumestrol with the targets was even higher than that for the corresponding inbuilt ligands.



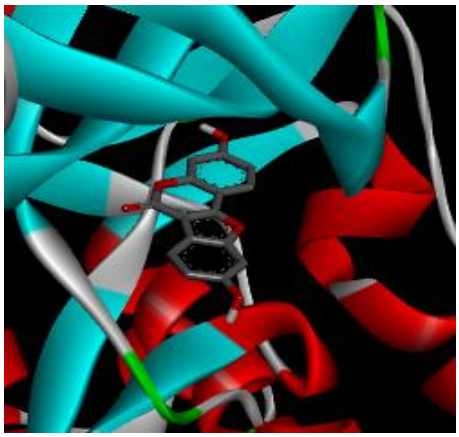


Fig. 1 Interaction of Coumestrol with JAK3

UNRAVELING THE INTERFACE CHEMISTRY OF ZnV_2O_6/g-C_3N_4 COMPOSITE APPLIED FOR VISIBLE-LIGHT-DRIVEN MINERALIZATION OF ANTIBIOTIC RESIDUE IN WATER

S. R. Yashas andH. P. Shivaraju

Department of Water & Health, JSS Academy of Higher Education & Research, Mysuru, Karnataka, India.

(Research Area: Polymers and Composite Materials)

Abstract: The present work validates the fabrication of asymmetrical zinc-vanadium oxide (ZnV_2O_6) embedded on graphitic carbon nitride (g-C_3N_4) composite for visible-light assisted photocatalytic degradation of tetracycline hydrochloride (TC), an antibiotic. The g-C_3N_4 was synthesized by pyrolysis of urea and ZnV_2O_6/g-C_3N_4 composite was prepared by hydrothermal process. The as-synthesized catalysts were subjected to scanning electron microscopy (SEM), Energy-dispersive X-ray spectroscopy (EDS), dynamic light scattering (DLS) analysis, X-ray diffraction analysis, Fourier-transform infrared (FTIR) analysis, and UV-visible spectroscopy to determine the morphological, configuration, and other intrinsic features. The 1:1 (ZnV_2O_6/g-C_3N_4) composite displayed the maximum TC degradation (87.2%) over the individual catalysts. The methodical investigations revealed that 20mg of 1:1 (ZnV_2O_6/g-C_3N_4) catalyst was ideal to decompose 20mg/L of TC with 9W of LED irradiation up to 125 minutes. The 1:1 composite retained its catalytic efficiency for three consecutive runs that mark its on-site application. The as-proposed system for TC degradation is promising for the construction of electronically compatible composite that results in slower recombination of charges and endorses rapid electron exodus within the composite, thereby fast-tracking the photodegradation.

Keywords: g-C_3N_4; ZnV_2O_6; photodegradation; LED light; tetracycline hydrochloride; environmental

remediation; organic pollutant.

STRUCTURAL, ELECTRONIC AND OPTICAL FEATURES OF $Be_xZn_{1-x}S$, $Be_xZn_{1-x}Se$ AND $Be_xZn_{1-x}Te$ ALLOYS- A DENSITY FUNCTIONAL BASED FP-LAPW STUDY

Utpal Sarkar[a, b] andSurya Chattopadhyaya[a]

[a] *Department of Physics, Tripura University, Suryamaninagar-799022, Tripura, India*

[b] *Department of Physics, Govt. Degree College, Kamalpur, Dhalai-799285, Tripura, India*.

(Research Area: Soft condensed matter)

Abstract: Structural, electronic and optical features of zinc-beryllium chalcogenide ternary alloys $Be_xZn_{1-x}Y$ (Y=S, Se, Te) have been computed employing density functional theory(DFT) based FP-LAPW approach. Structural features have been computed with WC-GGA functional and found that the lattice constant decreases, while bulk modulus increases nonlinearly with Be-concentration in each alloy system. The electronic properties are explored with the mBJ, EV-GGA and PBE-GGA functional and found that each ternary sample is a direct band gap (Γ-Γ) semiconductor. Band gap for each alloy system increases nonlinearly with Be-concentration *x*.In case of optical transitions, the chalcogen-p of valence band as initial states and Be-3s, 2p as well as Zn-5s states of conduction band as final states play the dominant role.In each alloy system, nature of variation of each of the static dielectric constant, static refractive index and static reflectivity with Be-concentration *x* is opposite, while critical point in each of the $\varepsilon_2(\omega)$, $k(\omega)$, $\sigma(\omega)$ and $\alpha(\omega)$ spectra with Be-concentration *x* is similar to the nature of variation of band gap with Be-concentration. Several calculated properties are found to agree well with the corresponding experimental findings.

Keywords: Zinc-Beryllium Chalcogenides, DFT, FP-LAPW, WC-GGA, TB-mBJ, EV-GGA, Electronic properties.

STUDY OF GROUND STATE PROPERTIES OF $MnTe_2$

Bhawana Thapa[1,2*],,Amit Shankar[1], P.K. Patra[2]

[1]*Condensed Matter Theory Research Lab, Department Of Physics, Kurseong College, Darjeeling, India.*

[2]*Department of Physics, North Eastern Hill University, Shillong-793022, India.*

(Research Area: Energy Materials)

Abstract: Transitional metal dichalcogenides have emerged as a family of crystals with great interest due to their intriguing properties and fundamental applications in technological field. We have used the full potential-linearized augmented plane wave (FP-LAPW) method to predict the electronic properties of $MnTe_2$. The density of states and energy bands of these materials suggest metallic nature of $MnTe_2$.. The analysis of the energy band structure reveals that the states near the Fermi energy level mainly consists of d-states of Mn with very little contribution from p-states of Te. The asymmetry seen in the spin up and spin down channels of pure $MnTe_2$ indicates the presence of magnetic moment and it also have a very high absorption coefficient, exceeding 10^4 cm^{-1}.

MONTE CARLO SIMULATION STUDY OF HYDROGEN STORAGE IN POROUS SLITS CARBON MATERIALS

Sudarsan Karki and Somendra Nath Chakraborty

Department of Chemistry, Sikkim University, Gangtok, Sikkim, India.

(Research Area: Energy Materials)

Abstract: Hydrogen is the best renewable, efficient and eco-friendly alternative energy power to replace the existing non-renewable and environmentally hazardous resources. The storage of molecular hydrogen as a fuel, meeting cost, saftey and performance are the major challenges faced by experimentalist and theoreticians. U.S. Department of energy sets target for different hydrogen storage systems keeping gravimetric density, volumetric density and cost into consideration[1]. We investigate the physisorption of hydogen in carbonaceous nanoslits of different sizes, based on Grand Canonical Monte Carlo (GCMC)[2] simulation technique. The three site model of hydrogen molecules, first proposed by Silvera-Goldman, in towhee it's defined by Alavi2005 potential was used. Simulation are performed at different temperatures in the range 60 -100 K and also at two additional teperatures 273 K and 298 K and corresponding hydrogen pressure are 0 bar, 5 bar, 10 bar, 30 bar, 50 bar, 100 bar, 200 bar, 300 bar, 400 bar and 500 bar. For all simulations one million, monte carlo steps were performed with a maximum 4,000 hydogen molecules were allows to fluctuate during simulation. The adsorption process have been studied considering, the adsorption capacities and energies, density profile and the effect of pore size under different conditions. Some of results we obtained were compared with literature data and found a good agreement.

References:

[1] Steven G Chalk and James F Miller. Key challenges and recent progress in batteries, fuel cells, and hydrogen storage for clean energy systems. Journal of Power Sources, 159(1) : 73–80, 2006.

[2] DJ Adams. Grand canonical ensemble monte carlo for a lennard-jones fluid. Molecular Physics, 29(1):307–311, 1975.

INCREASE OF MAGNETIC PARAMETERS IN SOL GEL PREPARED CuO:Fe:Nd Co-DOPED NANOPARTICLES

Albert Manoharan[1], R. Chandramohan[1,2], S. Valanarasu[3] and SR. Srikumar[4]

[1]*PG and Research Department of Physics, Sree Sevugan Annamalai College, Devakottai 630303, Tamilnadu, India*

[2]*PG Department of Physics, Vidhyaa Giri College of Arts and Science, Puduvayal-630108,Tamilnadu, India*

[3]*PG and Research Department of Physics, Arul Anandar College, Karumathur, Madurai - 625514, Tamilnadu, India*

[4]*Department of Physics, Kalasalingam Academy of Research and Education, Krishnankoil-626126,Tamilnadu, India.*

(Research Area: Condensed Matter Physics)

Abstract: Nanometer sized CuO materials are playing important role for the fabrication of next generation electronic circuits, magnetic and optoelectronic devices. Several metal oxide materials have been reported to reveal the ferromagnetic behaviour at room temperature, however the beginning of ferromagnetism is not fully understood because some of the intrinsic defects are produced in the dilute magnetic metal oxide materials during the synthesis process. Copper Oxide (CuO) materials have wide range applications such as gas sensors, solar cells and spintronics applications, etc. The CuO properties mainly depend on the intrinsic impurities and defects. We can reduce the defects of CuO lattice by the inclusion of various doping elements like transition metal ions (Fe) and rare earth metals (Nd, Gd, La). Because, the inclusion of rare earth (4f) and transition metal (3d) materials into the CuO lattice can supply a possible approach to establish the energy levels in the band gap variation. In this study, CuO nanoarticles were synthesized using sol gel method.Copper chloride dehydrate [Cu $Cl_2.2H_2O$], iron nitrate nanohydrate [$Fe(NO_3)_2.9H_2O$] and [$C_6H_8O_7$] were used as starting materialsUndoped (b) Fe doped (c) Fe, Nd co-doped ZnO nanoparticles were prepared under various dopant

concentrations.The structural, optical, morphological electrical and magnetic properties were studied and reported. The studies revealed the formation of monoclinic phase structure with typical JCPDS file No. 80-0076 and the samples have (-111) and (111) as preferred orientations. There was no Nd and Co related impurity phases were observed in XRD spectrum. It was confirmed that Fe and Nd elements were exactly included into the CuO lattice. The lattice parameters decreased slightly when the doped material Fe and co-doped material Nd were added with CuO. From the optical study, it was observed that the reduction of band gap happens after doping. The PL intensity studies supports the XRD results that the crystallite size decreased with the inclusion of dopants. The doping retained the phase with minor modification in the crystallite size. The morphology revealed agglomerated grains. The grain sizes varied. The increase in conductivity and ferromagnetism were observed due to doping while the undoped CuO nanoparticles were also magnetic. The co doping of 3% Ni and 3% Co produced the increased remenance and magnetic properties. The results were explained.

CuO nanopartivles exhibited ferromagnetism. When iron (Fe) is doped into CuO, ferromagnetic ordering improves at room temperature and this could be explained on the basis of hopping mechanism of Fe ions. Magnetic moment obviously rises with the addition of transition metal element, which assigned more ferromagnetic properties toFe-doped CuO nanostructures and also to the coexistence of Cu^{2+} and Fe^{2+} ions through the double exchange mechanism. The Fe and Nd co doping in CuO nonomaterials can further enhance the magnetic properties by a similar mechanism.

FERMI SURFACE AND LIFSHITZ TRANSITION IN KAGOME METAL

Alisha Budhathoki[1] and Madhav Prasad Ghimire[1,2]

[1]*Central Department of Physics, Tribhuvan University, Kirtipur, Kathmandu, Nepal.*
[2] *Leibniz Institute for Solid State and Material Research, IFW Dresden, Germany.*

(Research Area: Condensed Matter Physics)

Abstract: Application of magnetic field, external pressure and doping can cause change in topology of Fermi surface. Wide range of investigation is going on to study kagome lattice to create device with perfect conductivity. Here, we perform density functional calculation to study $ScFe_6Ge_4$, a kagome system, where we noticed the material to be ferromagnetic with a total magnetic moment of 12.12 μ_B/unit cell. We found the metallic nature where Fe-3d shows the highest contribution at Fermi level in total DOS. Hybridization between Fe-3d and Ge-4p is observed around Fermi level. The wannier fitting with the DFT calculations was performed to obtain wannier Hamiltonian to explore the Weyl points in $ScFe_6Ge_4$. Here by means of external pressure we intend to find the Lifshitz transition from type I to type II Weyl Semimetals.

Keywords: Kagome lattice, Density functional theory, Lifshitz transition

INVESTIGATION OF MOLECULAR PROPERTIES OF SOME FLUOROBENZENE DERIVATIVES APPLYING A NUMBER OF EXPERIMENTAL TECHNIQUES.

Manabindu Das[1]and S. Haldar[2]

[1]*Kurseong College, Kurseong, Darjeeling, West Bengal, India*

[2]*Department of Physics, North Bengal University, Siliguri, India*

(Research Area: Liquid Crystal and Solar Cell)

Abstract: The results of X-ray diffraction, dielectric spectroscopy and optical birefringence studies on nematogenicfluorobenzene derivatives are presented. The thermal stability of the compounds increases substantially as greater flexibility is introduced into the core structure. Average intermolecular distances, obtained from X-ray data, are found to increase when a comparatively rigid planar phenyl ring is substituted by a flexible non-planar cyclohexyl ring in the core structure. From the values of apparent molecular lengths in the nematic phase, a short range antiferroelectric type of association is found to exist between neighboring molecules. Molecular dipole moments have also been determined by measuring the dielectric constants and refractive indices of solutions of the compounds in a non-polar solvent p-xylene. Dipole moment of an isolated molecule is evaluated by extrapolation to infinite dilution. The calculated values of dipole moments were compared with our experimental data.

MULTI WALL CNT GROWTH USING WASTE PLASTIC AS CARBON SOURCE

Aunggat Shah and Mrityunjoy Mahato

Department of Basic Sciences and Social Sciences, School of Technology, North-Eastern Hill University, Shillong, India.

(Research Area: Nano and Biomaterials & Applications)

Abstract: Waste plastics have become a concern for the society due to its non-biodegradability. Researches is going on to minimize waste plastic and develop product out of plastic using cost effective methods. One of the routes is to grow carbon nanotubes (CNTs) using waste plastic as carbon source. Herein, we have suggested a cost effective metal oxide-CNT composite preparation method which can be further used for various applications. The methodologies involve preparation of metal oxide-NP catalysts by co-precipitation method using metal salts as reaction precursors. The catalysts were then used for direct preparation of CNT growth by pyrolysis of waste plastic in an electric furnace. The CNTs were grown with yield 10 wt%, having Raman I_D/I_G ratio of 0.90with diameter of 5 nm to 20 nm. UV-Vis spectra revealed a reduction in band gap energy with the formation of metal oxide composites as compared to metal oxides; indicating the presence of CNTs. XRD peak observed at $2\theta = 26^o$ is attributed to the formation of CNTs. Our study will open up new avenues for direct preparation of CNT-metal composite as an economically viable product from waste plastic recycling.

Keyword:CNT, Plastic Waste, Pyrolysis

Reference

[1] J. C. Acomb, C. Wu, P. T. Williams *Applied Catalysis B: Environmental* 147 (**2014**) 571–584.

[2] M. El-Kemary, N. Nagy, I. El-Mehasseb *Materials Science in Semiconductor Processing* 16 (**2013**) 1747–1752.

NOVEL TOPOLOGICAL WEYL SEMIMETALLIC PHASE IN LAYERED MATERIAL: Fe_2Sn

Bishnu Karki[1,,2], Bishnu Prasad Belbase[1,2], and Madhav Prasad Ghimire[1,2,3]

[1] *Central Department of Physics, Tribhuvan University, Kirtipur, 44613, Kathmandu, Nepal*

[2] *Condensed Matter Physics Research Center, Butwal-11, Rupandehi, Nepal*

[3] *Institute for Theoretical Solid State Physics, IFW Dresden, Helmholtzstr-20, 01069 Dresden, Germany*

(Research Area: Material Science)

Abstract: The result of crossing of the non-degenerate valence and the conduction band in the momentum space generates two folded degenerate nodes which are the sources for the masslessquasi-particles called Weylfermions. The materials hosting such nodes are the topological Weylsemimetals (WSMs) as the local perturbations do not open the gap of crossing instead can be moved within the brillouin zone. The huge applications in the field of quantum computing and the spintronics attracts the search for these fermions. Here we focus on studying the first principle calculation of the electronic, magnetic and transport properties of the layered material Fe_2Sn using Full Potential Local Orbital Code (FPLO). From our density functional theory calculations, the magnetic ground state is found to be ferromagnetic with a total magnetic moment of $9.12\mu_B$/ unit cell. The electronic state shows metallic behavior with the band crossing close to the Fermi level. Fe_2Sn is predicted to be magnetic WSMs based on the identification of Weylpoints close to the Fermi level with chirality ± 1. Moreover, the high peak values of anomalous hall conductivity are observed in the energy range of Weyl points.

Keywords: Weyl Semimetals, Density functional theory, Chirality

BROMOTHYMOL BLUE DYE/ PVA COMPOSITE FILMS: FACILE ECONOMIC AND FLEXIBLE LASER FILTERS

Debopriyo Ghoshal[1,2],Debopriya Bhattacharya[1], Dheeraj Mondal[3], SukhenDas[3], Navonil Bose[4] and Mousumi Basu[1*]

[1]*Department of Physics, Indian Institute of Engineering Science and Technology, Shibpur, Howrah-711103, India*

[2]*Future Institute of Technology, Garia, Kolkata- India*

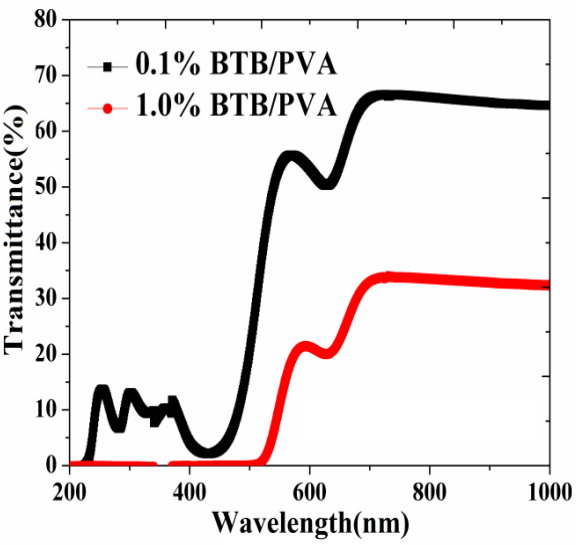
[3]*Department of Physics, Jadavpur University, Kolkata-700032, India*

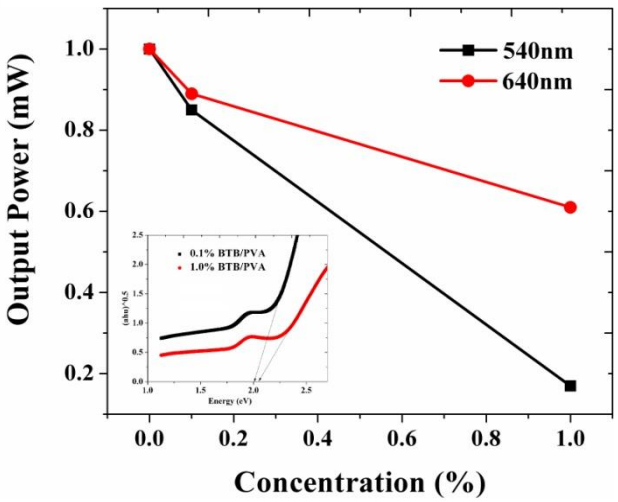
[4]*Department of Physics, Supreme Knowledge Foundation Group of Institutions, Mankundu, India*

(Research Area: Polymer and composite materials)

Abstract: Dye/polymer composite films are mostly useful as the most important segment of optoelectronic devices due to their excellent optical, mechanical and electrical properties. Here we study the structural and optical properties of the low-cost Bromothymol blue(BTB)/poly (vinyl alcohol) (PVA) composites (BTB concentration 0wt%, 0.1wt%, 1.0wt %) arranged by simplistic solution casting technique. A considerable change in the band gap is also observed for the 1.0% BTB/PVA composite (~2.1eV) than that of the neat PVA (~4.7eV). A 1.0wt% BTB/PVA film of width 250 ± 20 μm can fully block visible light in the 200-540nm wavelength region and can successfully block high power laser (2.1mW) of wavelength~540 nm.

Keywords: Dye-polymer Composite; Optical Properties; Laser cut-off Filter; band gap





Reference:

1. D. Ghoshal, D. Bhattacharya, D. Mondal, S. Das, N. Bose, M. Basu, (2019) Methylene Blue/PVA Composite Film for Flexible, Wide-scale UV–VIS Laser Cut-Off Filter, Mater. Res. Express, 6:075332.
2. D. Ghoshal, D. Bhattacharya, D. Mondal, S. Das, N. Bose, M. Basu, (2019) Flexible alizarin red/PVA composites with colossal dielectric and high power laser filtering properties, Applied Physics A, (2020) 126:28.
3. S. M. El-Bashir, I. S. Yahia, M. A. Binhussain, M. S. AlSalhi, (2017) Designing of PVA/Rose Bengal long-pass optical window applications, Results in physics, 7:1238-1244.
4. R. Bisen, J. Tripathi, A. Sharma, A. Khare, Y. Kumar, S. Tripathi, (2018) Optical behaviour of coumarin dye in PVA and PMMA film matrices,Vacuum,152:65-69.

STRUCTURED WATER CHAINS IN EXTERNAL ELECTRIC FIELDS

Smita Rai, Nayan Sharma & Dhurba Rai

Department of Physics, Sikkim University, Tadong, Gangtok, Sikkim, India.

(Research Area: Condensed Matter Physics)

Abstract: We study the structural, energetic and electronic properties of the structured water chain clusters within the density functional theory. We refer the structured water chains to those water clusters that have specific geometric patterns stretched along one direction. The structures are essentially periodic with basic repeating unit consisting of the corner- or edge-sharing 4-, 5- or 6-membered ring water clusters. We optimize the structures within the GAUSSIAN 16 suite of programmes in the presence of small electric fieldrequired to keep the structures open chain, thereby preventing them to form closed structures. We employ B3LYP functional with a standard basis set 6-311++G(d,p) for both geometry optimization as well as frequency calculations. We also employ other functionals, e.g. ωB97X-D, M06-2X suitable for non-covalent interactions, and the results are compared with the B3LYP calculations for pentamer chains. Analysis reveals that the pentamer chain clusters have the lowest average dipole moment per water molecule while the threshold field, that marks the onset of the field-induced closure of the HOMO–LUMO energy gap, is highest, followed by the tetramer and hexamer chains. The results suggest that the pentamer chains are the most stable clusters. The HOMO–LUMO energy gap decreases after reaching a maximum at the threshold field, while the average binding energy increases monotonically showing that there is no strong correlation between the chemical and energetic stabilities of the clusters under consideration.Our findings have important implications for device applications that exploit the structural behaviors and the associated properties of the structured water clusters.

CONSEQUENCES OF PI-ETA MIXING IN NUCLEAR MATTER

Subhrajyoti Biswas

Department of Physics, Rishi Bankim Chandra College, North 24 Parganas, West Bengal, India

(Research Area: Particle and Nuclear Physics)

Abstract: The present work studies two important consequences of pi-eta mixing in nuclear matter, particularly in asymmetric nuclear matter. The mixing of such isospin pure resonance states is driven by the asymmetry of the nuclear matter. First we explore the modification of the masses of mesons participating in the mixing and secondly the charge symmetry breaking in-medium interaction within the framework of one boson exchange model. We show that mixing reduces the in-medium mass of pion while increases the same of eta meson. We also construct the two-body charge symmetry breaking in-medium potential considering both the modification of nucleon and meson masses.

A SPECTROSCOPIC STUDY OF THE LOW REDSHIFT DWARF GALAXY SDSS J134326.99+431118.7 TO CALCULATE STAR FORMATION RATE

Daya Nidhi Chhatkuli[1], Sanjaya Paudel[2] and Binil Aryal[1]

[1]*Central Department of Physics, Tribhuvan University, Kirtipur, Nepal,*

[2] *Centre for galaxy evolution research (CGER), Department of Astronomy, Yonsei University, Seoul, South Korea*

(Research Area: Astrophysics and Space Research)

Abstract: We present a spectroscopic study of an interacting emission-line dwarf galaxy SDSS J134326.99+431118.7. We analyzed eight-strong emission lines of wavelength in a range of 3902.1Å to 6619.1Å. Among them, the strongest emission line is OIII, with an intensity of 1043.6 x 10^{-17} erg/s/cm^2/Å. These characteristic lines show a perfect Gaussian fit with a coefficient of regression greater than 98%, where the derived full width half maximum (FWHM) is less than 3.8 Å. The line ratio between H_α and H_β (H_α/ H_β)2.73. This suggests that the galaxy is a starburst galaxy. Star Formation Rate (SFR) of the galaxy derived from H□□ emission line flux is 0.019 $M_\odot year^{-1}$ and emission line metallicity derived from flux ratio between NIII and H□ □ □is 7.85 dex. These morphological and physical properties of SDSSJ134326.99+431118.7 are very similar to those of a typical Blue Compact Dwarf (BCD) galaxy. We conclude that we have presented another evidence of forming a BCD-type galaxy through a merger.

Keywords: Dwarf Galaxy, Star Formation Rate, Characteristics Peaks, H_α-line.

STUDY OF ELECTRONIC, MAGNETIC AND TRANSPORT PROPERTIES OF BaTbO3

Dhurba Raj Jaishi [1,2] and Madhav Prasad Ghimire[1,2]

[1]*Central Department of Physics, Tribhuvan University, Kirtipur, 44613, Kathmandu, Nepal.*
[2]*Condensed Matter Physics Research Center (CMPRC) Butwal,-11, Rupandehi, Nepal.*

(Research Area: Condensed Matter Physics)

Abstract: In this work we have investigated electronic, magnetic and transport properties of rare-earth ternary compound $BaTbO_3$ based on density functional theory using the generalized gradient approximation. This material is found to be ground state antiferromagnetic semiconducting in nature with energy gap 0.7 eV. The study of transport properties under constant relaxation time approximation ($\tau=10^{-14}$) and rigid band approximation in the temperature range 300-1200 K found large value power factor of 208 μW $cm^{-1}K^{-2}$ at 1200 K, which indicates the potential candidate for good thermoelectric material.

Keywords: Density Functional Theory, Thermoelectric, Power factor

FIRST-PRINCIPLE STUDY OF ELECTRONIC STRUCTURES OF COMPLEX TRANSITION METAL OXIDES: $CaVO_3$/$SrVO_3$

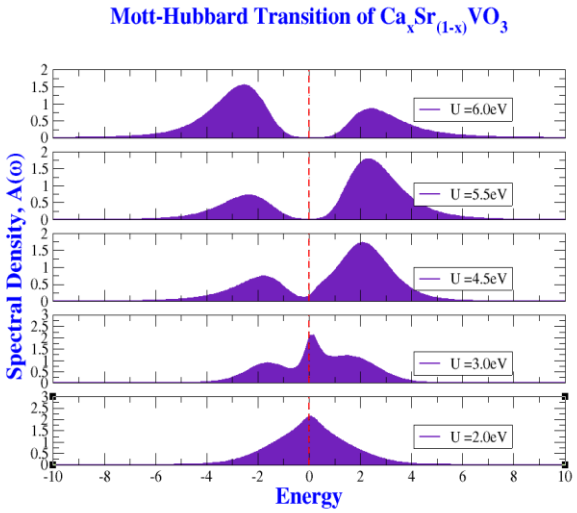
R. K. Rai[1] , G. C. Kaphle[1], O.P. Niraula[2]

[1]*Central Department of Physics, Tribhuvan University, Kirtipur, Kathmandu, Nepal*

[2]*Patan Multiple Campus, Tribhuvan University, Patandhoka, Lalitpur, Nepal*

(Research Area: Condensed Matter Physics)

Abstract: The most active area of research in the field of condensed matter physics is the strongly correlated electronic system, such as complex transition metal oxides (CTMOs) and their heterostructures in all dimensions.In this work, we have studied the electronic band structure and density of states (DOS) in cubic phase single crystals $CaVO_3$ and $SrVO_3$ using the density functional theory (DFT), within the generalized gradient approximation (GGA, GGA +U, GGA +U+J, GGA+SOC).The 2D and 3D charge density plot for $CaVO_3$ and $SrVO_3$ are done for finding the nature of bonding between the neighboring atoms of the system.



The long cherished dream of material scientists of tuning and tailoring transport properties of strongly correlated electron systems in a controlled fashion in their nano and bulk dimensions by varying carrier concentrations (creating vacancy or controlling the doping levels) counts as a tool to obtain high-temperature superconducting phases, a novel exotic physics such as insulator-metal transitions (IMT), colossal magnetoresistance (CMR), orbital- or charge-ordered (CO) or charge-disproportionate (CD) states.From this study, it is concluded that the role of unfulfilled d- and f- orbitals of transition

metals are crucial for tuning the electronic structure, transport properties, magnetic properties of TMO's, they are almost contributing on the Fermi-level of the bandstructure and plays role of itinerant or localized electrons depending on the strength of correlation effect.The ALPS-DMFT package and ABINIT package have been used for studying the DFT+DMFT calculation of heterostructure of (Ca,Sr)VO_3 as in fig.1.

Keywords: Complex TMOs, DFT+DMFT, GGA, Heterostructure, Strongly Correlated System

IDENTIFICATION OF HALF METALLICITY IN Co-DOPED $Rb_2Ni_3S_4$

Gang Bahadur Acharya[1] and Madhav Prasad Ghimire[1,2]

[1]*Central Department of Physics, Tribhuvan University, Kirtipur, 44613, Kathmandu, Nepal.*
[2]*Institute for Theoretical Solid State Physics, IFW Dresden, Helmhotzstrasse 20, 01069 Dresden, Germany.*

(Research Area: Condensed Matter Physics)

Abstract: $Rb_2Ni_3S_4$ is a Kagome system belonging to the space group Fmmm (Orthorhombic). Here we performed density functional theory (DFT) calculation using the full potential local orbital code (FPLO) and identified ferromagnetic ground state with low magnetic moment. We consider Co doping by replacement of Ni on $Rb_2Ni_3S_4$. Interestingly half metallic ferromagnetic behavior is observed with a total magnetic moment of 1.999 μ_B / unit cell. This indicates that the material is suitable spintronics device application in Kagome system.

Keywords: Kagome lattice, Density functional theory, Ferromagnetism

EFFECT OF THERMAL ANNEALING ON STRUCTURAL AND MICRO STRUCTURAL PROPERTY OF DC SPUTTERED TiO_2 THIN FILM

Haripriya Rath[1, 2], U.P. Singh[3] and N.C. Mishra[1]

[1]*Department of Physics, Utkal University, Bhubaneswar 751004, India*

[2]*College of Eng. and Tech., Techno Campus, Ghatikia, Bhubaneswar 751029, , India*

[3]*KIIT University, Bhubaneswar 751024, India*

(Research Area: Energy Materials)

Abstract: This study reportsfabrication of preferentially (101) oriented rutile TiO_2 filmon direct exposure of Titanium metal film to thermal oxidation. The films were deposited by DC magnetron sputtering from titanium target in pure argon gas atmosphere. The films were annealed at different temperatures between 100 and 1000 C in air for 1 hour. The structural, micro structural and optical properties of TiO_2 thin film are investigated byglancing angle X-Ray diffraction (GAXRD), Raman and atomic force microscopy (AFM) and UV- Visible spectroscopy. The as-deposited titanium thin film is amorphous, whereas the titanium thin film annealed at range of 400 - 1000C for 1h in air show rutile peaks in glancing angle X-Ray diffraction. The rutile crystallite size is found to increase from 27 nm in 400 C annealed film to 50 nm in 1000 C annealed film. Peaks due to the less stable anatase phase were not observed. The optical band gap is found to be 3 eV in case of the film annealed at 1000 C which matches with the band gap of bulk rutile phase. Like grain size, RMS roughness estimated from AFM study also found to increases exponentially with annealing temperature. The transformation from amorphous to rutile phase as seen in GAXRD study is also confirmed by Raman characterization. The present study has thus shown direct conversion of amorphous metallic titanium film to the most stable phase rutile TiO_2 on annealing at high temperatures without the formation of the intermediate anatase phase.

HIGH-PERFORMANCE THIN FILM SOLAR PV TECHNOLOGY IN CONTEXT TO INDIAN ENERGY SECTOR

[1]Ayan Banik

Department of Electrical Engineering, Cooch Behar Government Engineering College, India

(Research Area: Energy Materials)

Abstract: Indian renewable energy sector ranks fourth in global energy market although there is only 17-18% share of combined renewable energy as per the modern-day scenario. The growth is projected to be 175 GW capacity for the next substantial years i.e. 2021-2022 with a considerable progress percentage estimated to be 50-60% by International Renewable Energy Agency (IRENA). Among various green energies, solar energy has been identified as the most potential source and significantly characterized by its unique nature such as availability, reliability, adaptability, flexibility, efficient optimization, hazel free operation and most importantly almost free run charges with zero carbon footprint. Moreover, its application has been found throughout every corner of our society including scientific activities. Government of India has understood its growing importance and in turn, promotes the widespread adoption and sustainable usage of energy-efficient thin-film solar PV. In this work, the author has been involved in simulation, systematic performance analysis, case studies, validation, exploration of numerous scopes and possibilities of thin-film photovoltaics technology. A scientific approach through smart investigation has been adopted to accomplish reliable operation and advancement in thin-film technologies for their faster multidimensional adoption. Strategies have been proposed with the targeted sector which has a substantial role in India's energy sector in turn strengthening nation. The specific outcome has been observed and presented with highlighted future scope to emphasize thin photovoltaic technology to ensure a sustainable environment.

SYNTHESIS AND CHARACTERIZATION OF VISIBLE LIGHT ACTIVE $TiO_2/CoTiO_3$HYBRID NANOSTRUCTURE AND STUDY OF ITS CHARGE CARRIER TRANSFER DYNAMICS

Rajmoni Basumatary and Anjalu Ramchiary

Department of Physics, Bodoland University, Rongalikhata, Kokrajhar, Assam, India.

(Research Area: Condensed Matter Physics)

Abstract: The optical absorption and charge carrier transfer mechanism of hybrid structure of titania and cobalt titanate ($TO_2/CoTiO_3$) was investigated for potential applications in photocatalysis. Various characterization techniques were used to study the structural, optical and morphological properties of the material. Pristine TiO_2 and $TO_2/CoTiO_3$ samples were calcined at different temperature to study the structural and phase transformations. The UV-DRS spectrum of pristine TiO_2 shows an absorption spectra in the ultraviolet region corresponding to the bandgap of 3.2 eV. However, the band gap of the nanohybrid is found to be significantly less compared to the pristine TiO_2, which enunciates the formation of interstitial energy states due to colligation of TO_2 and $CoTiO_3$. The crystallinity and presence of both TO_2 and $CoTiO_3$ is confirmed by Powder X-ray diffraction (PXRD) spectra. The morphology of TiO_2 and $TiO_2/CoTiO_2$ were investigated using scanning electron microscopy (SEM) and transmission electron microscopy (TEM) technique. The average particle size is found to be 35 ± 5 nm which is consistent with PXRD results. The broad absorption spectra of the sample reveals the enhancement in the absorption of light in visible range, and the effective interfacial separation of the photogenerated charge carriers due to $TiO_2/CoTiO_2$ heterostructure may dramatically enhance the photocatalytic activity.

BIOSYNTHESIS OF GOLD NANOPARTICLES BY USING THE AQUEOUS LEAF EXTRACTS OF *ELAEOCARPUS SERRATUS*

Samiran Upadhyaya, Saponjeet Borah, Neelotpal Sen Sarma

Advanced Materials Laboratory, Institute of Advanced Study in Science and Technology, Paschim Boragaon, Guwahati, Assam, India.

(Research Area: Nanomaterials)

Abstract: In this work, we report the biosynthesis and characterization of gold nanoparticles of size around 8-10 nm. Gold nanoparticles were synthesized by using the aqueous leaf extract of *Elaeocarpus Serratus*, commonly called *Jolfai*,in the local language. The nanoparticles were prepared in different pH mediums and found that the basic medium results in the most efficient formation of nanoparticles. The nanoparticles were characterized using different spectroscopic techniques, such as UV-Visible spectroscopy, Fourier Transformed Infrared, Scanning Electron Microscope, and Transmission Electron Microscope. The nanoparticles do not get agglomeratedand were found to be stable for more than six months, without the use of any stabilizing agents. This process paved a new way to synthesize gold nanoparticles without the use of toxic reducing agents.

RECENT ADVANCES IN FLUORESCENT CARBON QUANTUM DOTS FOR WHITE LED APPLICATIONS

Varun D. Sharma and Milan Kumar Bera

Department of Physics, Maharishi Markandeshwar (Deemed to be University), Mullana Ambala (133207), Haryana, India.

(Research Area: Nanomaterials)

Abstract: Carbon quantum dots (CQDs), which are semiconducting nanocrystals, have attracted a lot of attention for their potential applications in various fields such as light-emitting diodes (LEDs), ion detection, bio imaging, solar technology, photocatalysis etc. CQDs are promising in optoelectronic applications especially in white-emitting diodes (WLEDs) for bright white light emission because of their characteristic broad emission, tunable fluorescence emission and high thermal stability. Carbon quantum dots are defined as a class of zero-dimensional (0-D) nanoparticles with ultrafine sizes of <10 nm, whose electronic bandgap structures are mainly influenced by the quantum confinement effect. This review updates on the recent advances in the design of high-performance WLEDs with diverse allied color temperature by tuning the red component using the red emissive CQDs and single-component white emissive CQDs. The advancement of CQDs based WLEDs with higher efficiency and color quality will also be discussed. Besides, room temperature phosphorescence and thermally activated delayed fluorescence are required for highly efficient WLEDs exploiting the properties of triplet-excited-state in CQDs. However, there is plenty of room for ground-breaking advances in both fundamental research and optoelectronic applications of CQDs in the near future.

Keywords: Carbon quantum dots; White light-emitting diode; Optoelectronic devices

MONITORING OF GEOMAGNETIC STORM INDUCED VLF SIGNAL DISTURBANCES FROM A LOW LATITUDE STATION AT COOCH BEHAR, INDIA

Kheyali Barman[1], Rajashree Nath [1], Arnab Sen [2], Bakul Das [1], Sujay Pal[3],Prabir Kr Haldar [1]

[1]*Department of Physics, Cooch Behar Panchanan Barma University, Vivekananda Street, Cooch Behar, West Bengal 736101, India*
[2]*Department of Education in Science and Mathematics, NERIE, NCERT, Shillong, Meghalaya 793103, India*
[3]*Department of Physics, Srikrishna College, Nadia, WB 741502, India*

(Research Area:Astrophysics and Space Research)

Abstract: A geomagnetic disturbance is observed between 26th and 27th August 2018due to persistent activity caused by the 20 August coronal mass ejection of Sun. The geomagnetic storm peaks at 0600 UT with geomagnetic indices *Kp* = 7, *Ap* = 154 and *Dst* = - 174 nT and lasts for 21 hours. VLF signals transmitted from the VTX transmitter [8.22°N; 77.75°E] at 18.2 kHz and the NWC [21.816^{0}S; 114.165^{0}E] transmitter at 19.8 kHz are being continuously received at Cooch Behar (CHB), India [26.334°N; 89.326°E]. Observation of VLF signal disturbances on both VTX and NWC signals shows that the signal amplitude of falls towards -3σ on 26 to 27 August in the night time, but stabilizes in the day time on 27th August and reaches minimum and crosses -3σ line in the night time on 27-28 August. On the other hand, night time amplitude of NWC signal of 26-27 August shows a fluctuation between ±3σ lines at around mid-night. NWC amplitude on the terminator just after 27th August (in the evening) shows a deviation towards -3σ but in the night time the data looks undisturbed. Both these dipping of VTX and NWC signal amplitudes at night coincide with the storm occurrence period or in the storm recovery phase. Interestingly, VTX amplitude after the evening terminator of 28th August enhanced and crosses +3σ line, which is not available on the NWC signal. That may be due the Travelling Ionospheric

Disturbances in the storm recovery to the quite conditions. This kind of observation is clearly encouraging to monitoring of geomagnetic storm using VLF remote sensing.

References

[1] Kikuchi, T., and D., S., Evans, 1983. Quantitative study of substormassociated VLF phase anomalies and precipitatingenergetic electrons on November 13, 1979 *J. Geophys. Res.,* 88, 87

[2] K., Tatsuta, Y., Hobara, S., Pal, and M., Balikhin, 2015. Sub-ionospheric VLF signal anomaly due to geomagnetic storms: Astatistical study *Ann. Geophys.*, 33, 1457–1467, 2015 www.ann-geophys.net/33/1457/2015/ doi:10.5194/angeo-33-1457-2015

[3] Kumar, A., Kumar, S., 2014. Space weather effects on the low latitude D-region ionosphere during solar minimum. *Earth Planet Sp* 66, 76. https://doi.org/10.1186/1880-5981-66-76

BISMUTH DOPED COBALT CHROMATES NANOPARTICLES: A DETAILED STUDY OF STRUCTURAL, MICROSTRUCTURAL, ELECTRICAL AND MAGNETIC PROPERTIES

K. Manjunatha[1], V. Jagadeesha Angadi[2],U. Mahaboob Pasha[1,3]

[1]*Department of Physics, School of Engineering, Presidency University, Bangalore-560064, India*

[2]*Department of Physics, P.C. Jabin Science College, Hubballi-580031, India*

[3]*Faculty of Material Science and Metallurgy, South Ural State University, Chelyabnisk, Russia*

(Research Area: Condensed Matter Physics)

Abstract: In the present work, the $Co_{(1-x)}Bi_xCr_2O_4$ (where x = 0.00, 0.05, 0.10) nanoparticles have been synthesized by solution combustion method. The $Co_{(1-x)}Bi_xCr_2O_4$ (where x = 0.00, 0.05, 0.10) nanoparticles are studied through structural, microstructural, electrical and magnetic properties. Structural analysis, average crystallite size and lattice parameters were done by X-ray diffraction (XRD). The refined XRD pattern of all the samples confirms a single-phase formation without any secondary peak.confirms the porous nature of the samples and elemental analysis were done by using Scanning electron microscopy (SEM) and Energy dispersive X-ray spectroscopy (EDS) respectively. Particle size of the samples were estimated by Transmission electron microscopy (TEM). The activation energy of the samples was estimated by using DC conductivity measurements. The DC conductivity increases with temperature were explained by percolation theory. At 300 K, M-H loop shows a paramagnetic behaviour for all samples. At 95 K, M-H loop shows a slim S type of hysteresis loop and it confirms the ferrimagnetic nature. At 25 K, M-H loop shows a hysteresis loop with remanent magnetization and coercive field. The magnetic properties of the all samples was concentrated through susceptibility as a function of temperature and we watch two magnetic transitions, for example, paramagnetic to long range

collinear ferrimagnetism transition at curie temperature and non collinear ferrimagnetism at spiral transition temperature.

Keywords: *Ferrimagnetic transition; Susceptibility; Transmission electron microscopy; Solution combustion method.*

STELLAR SCINTILLATIONS AND OCCULTATION: AN ASTROPHYSICAL APPROACH TO THE GUIDING TURBULENCE IN TROPICAL CYCLONES

Indrajit Ghosh[1], Sukhen Das[2] and Nabajit Charravarty[3]

[1]*Deptartment of Physical and Material Science,College of Engineering and Management, Kolaghat, East Medinipur, West Bengal, India.*

[2]*Dept. of Physics, Jadavpur University, Kolkata, West Bengal, India.*

[3]*Positional Astronomy Centre, Plot No.8, Block-AQ, Sector-V, Salt Lake City,West Bengal, India*

(Research Area: Astrophysics)

Abstract: For the past three decades the frequency and intensity of tropical cyclones have greatly increased resulting in considerable devastation to the coastal fraternity throughout the World. In general, satellite imaging observations, Doppler radar data, Reconnaissance flight data record, RSRW data analysis etc. scientific meteorological techniques are used for the prior forecasting of tropical depressions over ocean bed that results in the generation of tropical cyclones. Apart from these, some advanced conventional meteorological techniques are also used to detect the path of propagation of tropical cyclones on landmass after their generation from depressions over ocean bed. But nowadays we need to focus on some more unconventional yet effective scientific techniques for the forecasting of tropical cyclones by studying the atmospheric turbulence pattern involved in tropical cyclone dynamics. With that objective we investigated the stellar scintillation and stellar occultation during occurrence of tropical cyclones. The radiation energy obtained from these astrophysical incidents possesses an important relationship with the vertical temperature profile during occurrence of a tropical cyclone. In fact, atmospheric turbulence parameters can be investigated from studying the parameters like wavelength, energy, intensity etc. of astrophysical radiations. These can be analogically equated as studying of crystal structure by investigating its subsequent X- ray diffraction pattern. We have utilized Kolmogorov turbulence theory to derive the relationship between stellar

scintillation radiation energy and subsequent temperature of cyclone vortex by analyzing the RSRW data for different cyclones that has hit the Coromondol coast in recent past. This work emphasizes the practical use of astrophysical observations for detecting the turbulence pattern of tropical cyclones for better cyclone path detection.

DIAMETER AND ATOMIC STRUCTURE DEPENDENT STRUCTURAL AND ELECTRICAL PROPERTIES OF ZIGZAG ZnTe NANOTUBES

Monoj Das[1] and Bikash C Gupta[2]

[1]*Department of Physics, Gushkara Mahavidyalaya, Purba Bardhaman, 713128, India*

[2]*Department of Physics, Visva-Bharati, Santiniketan, 731235, India*

(Research Area: Nano and Biomaterials & Applications)

Abstract: The study of the properties of nanomaterials is one of the thrust areas of research in the field of nanoscience attributed to their interesting properties which are appropriate for various technological applications. The nanomaterials of various dimensions include quantum dots, nanosheets, nanowires and nanotubes. These nanomaterials may be used as building blocks for the development of technological devices. Among the studies on nanomaterials, the research activity in the field of carbon based nanotubes accelerated tremendously after the synthesis of carbon nanotubes by IIjima [1]. Among non-carbon materials, ZnTe, a group II-VI compound semiconductor with a band gap of 2.2-2.3 eV, displays low resistivity, large transparency in visible light spectra. These properties make ZnTe a promising chalcogenide material for potential applications in photovoltaic devices, solar cells, green light emissions, photodetectors and lasers.

Using density functional theory based VASP [2] package, we report structural and electrical properties like wall thickness, binding energy, band-gap energy, work function etc of various zigzag ZnTe nanotubes. We observe that the binding energies of the nanotubes increase with tube diameter. On the other hand, wall thickness, band-gap and work function decrease with increasing tube diameter. We find that the band-gap may be varied from 2.042 eV to 2.281 eV and from 0.501 eV to 0.772 eV. These findings are useful in band gap engineering. The work function of the nanotubes may also be tuned from 5.825 eV to 5.523 eV and from 4.681 eV to 5.022 eV respectively by changing parameters such as diameter and atomic arrangement of the

tubes. These results may be useful in designing various field emission devices using ZnTe nanotubes.

References:

[1] S. Iijima, Nature **354** (1991) 56.

[2] G. Kresse, and J. Hafner, Phys. Rev. B **47** (1993) 558.

THE SCIENCE BEHIND THE UNSUNG INDIAN MUSICAL DRUMS

Amitabha Bhattacharyya
Department of Physics, Sikkim University, Tadong, Gangtok, Sikkim, India

(Research Area: Acoustics)

Abstract: The Indian sub-continent has a kind of traditional drums which are very special. Usual drums, like the western drums, and Indian drums e.g. *Dhak*, *Dhol*, *Dholak* etc. produce sound which is not pleasant to the ear. The reason is that a vibrating stretched membrane produces sound of frequencies not related as harmonics. These are instruments of indefinite pitch and can be used only to provide a rhythm.

On the other hand, there are the special drums, which may be called Musical Drums, like *Mridangam, Pakhawaj,Tabla,Khol, Pung, Naal, Dhimay,Sri LankanDholki* and our own *Madal*. The membrane of these instruments is weighted at a certain point which makes it produce a sound with frequencies that are related to each other in ratios of small numbers, making the sound pleasant to the ear, just like string instruments. These are instruments of definite pitch. Classical music in India is incomplete without at least one such instrument.

I will explain the differences between the classes of drums from the scientific point of view, along with the story of the construction and possible development of these drums.

INVESTIGATION OF GROUND STATE PROPERTIES OF TERNARY CHALCOPYRITE, CuXY2(X=Al, Ga,In; Y=S,Se)USING DFT

Nakul Chhetri[1], Amit Shanker[2], PK Mandal[2], PC Barman[1]

[1] *Department of Physics, Raiganj University, West Bengal, India*

[2] *Department of Physics, North Bengal University, West Bengal, India*

(Research Area: Condensed Matter Physics)

Abstract: The ternary chalcopyrites of the general formula CuXY2(X=Al,Ga, In; Y=S,Se) are widely studied due to their potentials as an alternative source of energy. In thispaper, the ground state properties of these crystals have been studied under the formalism of DFT. FPLAPW method incorporated within Wien2k code has been used with GGA(PBE) and LDA as exchange correlation potential. The geometrical parameters like lattice parameters are in close approximation with experimental values. The band structure, DOS and optical properties have also been studied. From the study we concluded that they direct band gap crystals. All results are in close approximation with existing results and experimental values.

FLAT BAND AND HALF METALLICITY IN KAGOME MAGNET $Y_{1-x}Ca_xCo_5$

Nileema Sharma [1,2] and Madhav Prasad Ghimire[1,2]

[1] *Central Department of Physics, Tribhuvan University, Kirtipur, 44613, Kathmandu, Nepal.*

[2] *Condensed Matter Physics Research Center, Butwal-11, Rupendehi, Nepal*

(Research Area: Condensed Matter Physics)

Abstract: The presence of robust flat band and high Magnetocrystalline Anisotropy Energy (MAE) in YCo_5, shows the typical nature of $RE(TM)_5$ having highest value of MAE among the mishmetals of similar nature. This system is pseudo-two dimensional ferromagnetic in nature. This makes it a potential candidate of permanent magnet. By doping hole (Ca) to the Y-site, the smaller ionic radii of Ca is found to enhance the MAE by making the alignment of easy direction of magnetization more easy, which in turn increases MAE. With Ca doping the original flat band is extended to whole Brillouin zone by shifting the Fermi level. This enables to control the filling of flat band upon doping, resulting in novel feature of band engineering.

Keywords: Itinerant magnetization, Kagome, Half-metal, Density Functional Theory (DFT)

ELECTRONIC AND MAGNETIC PROPERTIES OF BiTeI

Nirmal Saud[1] and Madhav Prasad Ghimire[1,2]

[1]*Central Department Of Physics, Tribhuvan University, Kirtipur, Kathmandu, Nepal*

[2]*Condensed Matter Physics Research Center (CMPRC), Butwal,-11, Rupandehi, Nepal.*

(Research Area: Condensed Matter Physics)

Abstract: There has been increasing interest in phenomena from relativistic electrons in a solid, which have a potential impact on spintronics and magnetoelectronics. We have studied the electronic and magnetic properties of BiTeI by means of full-potential linearized augumented plane wave method based on density-functional theory. In relativistic calculation the band gap is found to be 0.432 eV but non-relativistic calculation band gap is 1.273 eV. Hence in this calculation non-relativistic band gap is much greater than that of relativistic band gap due to spin-orbit coupling. Total density of states (DOS) and partial DOS have been computed.

CONSEQUENCES OF Ni DOPING ON THERMOELECTRIC PROPERTIES OF Bi_2Te_3

Labanya Ghosh[1] and Sandip Chatterjee [1]

[1]*Department of Physics, Indian Institute of Technology (BHU) Varanasi 221005, India*

(Research Area: Magnetic Materials and Spintronics)

Abstract: In order to study the thermoelectric properties of Ni doped Bi_2Te_3 compounds, the desired materials were synthesized by melt growth process. X-Ray diffraction pattern confirmed that the obtained crystals were easily cleaved along (00L) plane direction. Thermoelectric properties were investigated evaluating the absolute values of Seebeck coefficient. Temperature dependency of Seebeck coefficient indicated the changeover in carrier type as a result of Ni doping in Bi_2Te_3.

Keywords: Thermoelectric properties, Topological Insulators

ELECTRONIC AND MAGNETIC PROPERTIES OF DOUBLE PEROVSKITE Tb_2FeCrO_6

Sarita Lawaju,[1,2] Shalika Ram Bhandari,[1,2] and Madhav Prasad Ghimire[1,2]

[1]*Central Department of Physics, Tribhuvan University, Kirtipur, 44613, Kathmandu, Nepal*

[2]*Condensed Matter Physics Research Center, Butwal-11, Rupandehi, Nepal*

(Research Area: Condensed Matter Physics)

Abstract: The magnetic behavior of a compound can be understood in depth with help of the exchange interaction between 3d – elements, namely 3d – Fe and 3d – Cr, and their moments. The electronic and magnetic properties of Tb_2FeCrO_6 was investigated in order to explore the exchange interactions and their magnetic behavior. Density Functional Theory (DFT) calculation confirmed anti-ferromagnetic arrangement AFM2-↑↓↑↓ as ground state configuration with a band gap of 0.048 eV (2.372 eV) within GGA (GGA + U).

Keywords: Double Perovskite, Exchange coupling, Anti-ferromagnet

NATURALLY DERIVED BIOCOMPATIBLE FLUORESCENCE CARBON QUANTUM DOTS FOR *IN VIVO*TARGETING AND IMAGING OF TUMOR CELLS

Neetu Sharma[1], Indu Sharma[2], Tulshi Chakraborty[3], Milan Kumar Bera[1]

[1]*Department of Physics, Maharishi Markandeshwar (Deemed to be University), Mullana Ambala (133207), Haryana, India.*
[2]*Department of Biotechnology, Maharishi Markandeshwar (Deemed to be University), Mullana Ambala (133207), Haryana, India.*
[3]*Department of Pharmacy, Maharishi Markandeshwar (Deemed to be University), Mullana Ambala (133207), Haryana, India.*

Abstract: The early diagnosis and treatment of tumor remains a key challenge forbiomedical technology until today.Real-time imaging and targeting delivery have been the hot topics in cancer diagnosis and therapy. Developing nanomaterials for tumor labelling and therapy has been proposed to overcome the problems of complicated syntheses, expensive precursors, and emission losses, which are the major factors preventing the specific targeting of tumor cells instead of normal cells.The development of eco-friendly and nontoxic nanomaterials has becoming the key issues for *in vivo* targeted tumor cell imaging. In this regard, carbon based quantum dots (CQDs) have attracted attention because of its non-toxic, biocompatible andbiodegradable properties, such that it can be attached to drug/gene carriers. Therefore, this study reports on the facile green synthesis of naturally derived fluorescence CQDs. Fenugreek (*Trigonella foenum-graecum*) which is an annual herb in the family of *Fabaceae* has been chosen as precursor to drive CQDs using microwave-assisted synthesis (900 watt, 2.45 GHz). The hydroxyl & carboxyl groups present in CQDs are not only non-toxic to a wide range of cell lines, but also provide suitable surface chemistry for attachment to the specific drug for tumor cell treatment. This CQD-drug conjugate while injected into targeted tumor cell will provide *in vivo* fluorescence images under excitation in ultra-violet light.

Keywords: carbon quantum dots, drug delivery, *in vivo* tumor cell imaging.

DFT STUDY OF LIQUID CRYSTAL MATERIALS

Shivani Chaudhary

Department of Physics, , Babasaheb Bhimrao Ambedkar University, Lucknow (U.P.),India

(Research Area: Liquid Crystals)

Abstract: Liquid crystals (LCs) are a state of matter which has properties between those of conventional liquids and those of solid crystals. For instance, a liquid crystal may flow like a liquid, but its molecules may be oriented in a crystal-like way. There are many different types of liquid-crystal phases, which can be distinguished by their different optical properties (such as textures). The contrasting areas in the textures correspond to domains where the liquid-crystal molecules are oriented in different directions. Within a domain, however, the molecules are well ordered. LC materials may not always be in a liquid-crystal state of matter (just as water may turn into ice or water vapor). Liquid crystals can be divided into thermotropic, lyotropic and metallotropic phases. Thermotropic and lyotropic liquid crystals consist mostly of organic molecules, although a few minerals are also known. Thermotropic LCs exhibit a phase transition into the liquid-crystal phase as temperature is changed. Lyotropic LCs exhibit phase transitions as a function of both temperature and concentration of the liquid-crystal molecules in a solvent (typically water). Metallotropic LCs are composed of both organic and inorganic molecules; their liquid-crystal transition depends not only on temperature and concentration, but also on the inorganic-organic composition ratio.

THE STUDY OF STRUCTURAL AND DYNAMICAL PROPERTIES OF HEAVY WATER (D2O) PASSING THROUGH CARBON NANOTUBES

Shyam Sundar Sharma

Central Department of Physics, Tribhuvan University, Kirtipur, 44613, Kathmandu, Nepal

(Research Area: Nano and Biomaterials & Application)

Abstract: Structural and dynamical properties of water within carbon nanotubes are of great interest in recent technology because of its variety of applications in the area of nanoelectronics, optics, material science, mechanical, and biological fields. In this work, we have performed the Molecular Dynamics simulation to investigate the structure and dynamic properties of heavy water (D_2O) confined inside (6, 6) single-walled carbon nanotubes(SWCNT) and compare them to the normal water properties. For MD simulations the force field parameters of the D_2O water model were re-parameterized from the TIP3P water model in which we have doubled the mass of the hydrogen atoms and adjusted the partial charges of both the deuterium and oxygen atoms.

The simulation revealed that the CNTs can allow only a single file of water molecules. The water molecules inside the nanotubes show solid-like ordering at room temperature, which we analyze from the plot of radial distribution functions. Similarly, the diffusive behaviour of D_2O molecules has been investigated by means of the MSD plot exploiting Einstein's relation. The diffusion coefficient of D_2O is found to be $6.48\times10^{-5} cm^2/s$ which is about 12% lower than that of H_2O ($7.35\times10^{-5} cm^2/s$), which is in fair agreement with the experimental and theoretical data. Further, this study reports the permeation of D_2O molecules (i.e. 148) and found that observed permeation event is about 9% lower than that of H_2O (i.e. 164).

ECOFRIENDLY ZIRCONIUM MOF AND GRAPHENE BASED NANOHYBRID FOR DEGRADATION OF PHARMACEUTICAL DRUG FROM WASTEWATER

U. J. Vedash, Surinder Singh and Sushil Kumar Kansal

Dr. S. S. Bhatnagar University Institute of Chemical Engineering and Technology, Punjab University, Chandigarh

(Research Area: Nano and Biomaterials & Application)

Abstract: The release of pharmaceutical drugs in water bodies is a grave problem and concern for the environment. Many pharmaceutical drugs such asofloxacin, ketorolac tromethamine and levofloxacin are being used as antibiotics and anti-inflammatory drugs.The release of these antibiotics and pain killers to the aquatic environment is very harmful for the aquatic species.To degrade such environmental pollutants from water/wastewater many techniques and nanomaterials have been employed. Adsorption is a very useful and commonly employed technique due to its ease of operation and simplicity. The use of metal organic frameworks (MOFs) and nanocomposites have been employed to effectively degrade or remove these pharmaceutical contaminants from water bodies. Eco-friendly graphitic carbon nitride (g-C_3N_4) doped g-C_3N_4/UiO-66 nanohybrid (on a zirconium MOF, UIO-66) was utilizingin this study to remove synthetic drug ketorolac tromethamine from waste water. The lab made nanohybrid was characterized usingvarious analytical techniques. The as synthesized nanohybrid exhibited great adsorption capacity and could remove 80-82% ketorolac tromethamine drug from wastewater.

Keywords: Graphatic carbon nitride, environment pollutants, nanohybrid, pharmaceutical drug, adsorption, wastewater.

STUDY OF DEFORMATION BEHAVIOUR OF METALLIC NANOWIRES BY USING MULTI-SCALE COMPUTATIONAL MODELLING

Anirban Das

College of engineering and Management, Kolaghat, WB, India

(Research Area: Nanomaterials)

Abstract: With increasing miniature electronic device applications, nanowires become more and more important, as they have extraordinary mechanical strength and electrical properties, in compare to the bulk counter parts. The metallic nanowires show promising good results to form a touch-screen mesh over conventional ITO screens. In this present study, the yield strength of the same shaped different metallic nanowires has been studied in detail by using multi-scale computational modelling. All the systems (unit cells) were optimised to their ground state energies and lattice parameters by using conventional quantum density functional theory code (Quantum Espresso software).The optimized geometry gives you the strain free lattice constants, atomic coordinates, and the ground state crystal structure. Then the optimised data were feed to the standard molecular dynamical code (LAMMPS software). The computational techniques based on the molecular dynamics simulations provide an effective mean to understand the mechanical deformation behaviour of the nanowires with sufficiently high predictability and accuracy. The effect of uniaxial strain rate and temperature on the yield strength of the nanowires has been studied in detail. It is observed that for the higher strain rates the rate of dislocation generation is faster than the rate of dislocation annihilation. This leads to material hardening which causes the nanowires strength to increase. When the strain rate is increased, the yield stress and the fracture strain also

increased concurrently. But the yield strain does not seem to depend significantly on temperature.

Keywords: nanowires, quantum density functional theory (DFT), Molecular dynamics (MD) simulation

Indirect Calculation of Elastic Modulus of CNT Composites

Subhabrata Senapati[1], Aunggat Shah[1], Mrityunjoy Mahato[1,*], P. K. Patra[2]

[1]*Department of Basic Sciences and Social Sciences, School of Technology, North-Eastern Hill University, Shillong, India.*

[2]*Department of Physics, School of Physical Sciences, North-Eastern Hill University, Shillong, India.*

Abstract: In general, CNT composites are known to have extraordinary mechanical properties such as elastic modulus (E), tensile strength etc. However, due to its small size and destructive nature of mechanical property experimentation, researchers have attempted to develop an indirect method to calculate the value of E of CNT-composites. Fagergren et al. [1] haveproposed a model to calculate E in terms of density and Raman D-peak as main parameters. We adopted this model for NiO-MWCNT composites, which was prepared by pyrolyzing waste plastic and NiO as a catalyst. The Raman spectrum and TEM image data were also fed into the model. The obtained value of E from this model was found to be 8.3164 GPa which is well in the range of literature value of 62 MPa to 0.9 TPa [2]. Our work suggests that the model can be replicated to other different types of MWCNT composites.

Keywords: MWCNT-Composites, Elastic modulus, Raman spectroscopy.

Reference

[1] Fred Fagergren, Shane Sypherd, Dan Snow, Andrew Cunningham, and Brian Jensen. J. Micromech. Microeng. **29** (2019), 115015.

[2] Kadambinee Sa, Prakash Chandra Mahakul, Sunirmal Saha, Prakash Nath Vishwakarma, Karuna Kar Nanda, Pitamber Mahanandia. Polymer Engineering and Science, **59** (2019), 1075-1083.

ELECTRONIC PROPERTIES OF TOPOLOGICAL INSULATOR:BiSb

Sudeep Jnawali[1,2]and Madhav Prasad Ghimire[1,2]

[1]*Central Department of Physics, Tribhuvan University, Kirtipur, 44613, Kathmandu, Nepal.*

[2]*Condensed Matter Physics Research Center (CMPRC), Butwal-11, Rupandehi, Nepal.*

(Research Area: Condensed Matter Physics)

Abstract: Topological insulator (TI) has became one of the significant material in the field of solid state physics. We perform density functional calculations within the framework of Generalized Gradient Approximation to study electronic properties of topological insulator. The material under study is non magnetic having band gap 0.120 eV without considering the spin-orbit coupling (SOC). We found strong effect of SOC in this material, as this band gap disappear when we consider the SOC which clearly indicates that this material could be the best candidate for TI. We found main contribution from Bi-6p and Sb-5p near the Fermi level which are responsible for electronic properties of this material.

Keywords: Topological insulator, Density functional theory

ELECTRONIC AND THERMOELECTRIC PROPERTIES OF $CoTa_2O_6$

Sujit Bati[1,2], Bishnu Prasad Belbase[1,2], Hari. S. Nair[3] and Madhav Prasad Ghimire[1,2,4]

[1]*Central Department of Physics, Tribhuvan University, Kirtipur, 44613, Kathmandu, Nepal.*

[2]*Condensed Matter Physics Research Center, Butwal, Rupandehi, Nepal*

[3]*Department of Physics, 500 W University Ave, University of Texas at El Paso, El Paso, Texas 79968, USA*

[4]*Institute for Theoretical Solid State Physics, IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany*

(Research Area: Computational Condensed Matter Physics)

Abstract: We present the electronic and thermoelectric (TE) properties of $CoTa_2O_6$ compound which is a trirutile oxide and has space group P42/mnm. In this study, the electronic and TE properties of $CoTa_2O_6$ have been investigated by using density functional theory and Boltzmann transport calculations. We found $CoTa_2O_6$ to be a semiconductor with a band gap of ~0.41 eV. A maximum power factor (PF) of 1.6×10^{15} μW/(K^2 s cm) at 300 K was observed. The value of PF is coupled to the relaxation time of the charge carriers. Assuming a constant relaxation time of 10^{-15} seconds, the maximum ZT value achievable by electron doping is about 0.032 at 300 K. This value is very much smaller compared to the ZT values of state of the art TE materials.

A LOW-COST RECHARGEABLE AQUEOUS ALUMINUM-GRAPHITE BATTERY

Sunny Nandi andShyamal K. Das

Department of Physics, Tezpur University, Assam 784028, India

(Research Area: Energy Materials)

Abstract: Rechargeable batteries based on largely earth abundant elements hold immense promise in achieving high energy/power and ultra-durable energy storage device. A recent example is the chloroaluminate electrolyte based Al-ion battery with graphene cathode.[1] However, certain demerits of chloroaluminate electrolytes such as high reactivity to most of the metals, moisture sensitivity and high cost will be impediments for mass-scale production of Al-ion battery.[1-3] Utilization of water based electrolyte in rechargeable Al battery is expected to mitigate these challenges. Herein, for the first time, we report here the working of a rechargeable aqueous aluminum-graphite battery by electrochemically pairing metallic aluminum anode with exfoliated graphite cathode. A discharge potential of 1.8 V and cycling stability over several cycles is obtained.[4]

References:

[1] Eftekhari, A.; Corrochanoc, P. Electrochemical energy storage by aluminum as a lightweight and cheap anode/charge carrier. *Sustainable Energy Fuels* **2017**, **1**, 1246-1264.

[2] Das, S. K.; Mahapatra, S.; Lahan, H. Aluminium-ion batteries: developments and challenges. *J. Mater. Chem. A* **2017**, *5*, 6347-6367.

[3] Lin, M. C.; Gong, M.; Lu, B.; Wu, Y.; Wang, D.Y.; Guan, M.; Angell, M.; Chen, C.; Yang, J.; Hwang, B. J.; Dai, H. An ultrafast rechargeable aluminium-ion battery. *Nature* **2015**, *520*, 325-328.

[4] Nandi, S.; Das, S.K. Realizing a low cost rechargeable aqueous aluminum-metal battery with exfoliated graphite cathode. *ACS Sustainable Chem. Eng.***2019**,*24*, 19839-19847.

DEVELOPMENT OF LOW TEMPERATURE SURFACE PASSIVATION AND ANTIREFLECTION COATING FOR SINGLE AND MULTICRYSTALLINE SILICON SOLAR CELL

Tapati Jana [a,*], Kuntal Biswas [b], Romyani Goswami[c] and Swati Ray[d]

[a]*Department of Physics. Sarojini Naidu College for Women, 30 Jessore Road, Kolkata 700 028, India*

[b]*Department of Physics. Dum Dum Motijheel College, Dumdum, Kolkata 700 074, India*

[c]*Department of Physics, Surya Sen Mahavidyalaya, Surya Sen Colony, Siliguri 734004, West Bengal, India.*

[d]*Energy Research Unit, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 70032, India*

(Research Area: Energy Materials)

Abstract: Low temperature surface passivation layer is one of the main challenge for further improvement of single and multicrystalline silicon solar cells. High temperature (~1000°C) thermally grown silicon oxide is an excellent surface passivation layer both n-type and p-type high resistivity wafers [1]. However, it causes compressive stress due to mismatch in thermal expansion coefficients between the substrate and the film, reduces bulk minority carrier lifetime. In this work, amorphous silicon oxide (a-SiO_x:H) and silicon nitride (a-SiN_x:H) layers are deposited at very low substrate temperature of 250 ^oC -300^oC by chemical Vapour deposition. Interface charge density (D_{it}) and fixed charge density (Q_f) have been estimated by high frequency (1 MHz) capacitance-voltage measurement on Metal–Insulator–Silicon structure (CV-MIS). The low interface charge density (D_{it}) reduces the surface recombination velocity. Fixed positive charges (D_f) stored in SiO_x:H/a-SiN_x:H layer form negative charges at silicon film. The band bending due to negative charges provides a very effective field induced surface passivation. A significant improvement in efficiency and short circuit current has been observed using developed a-SiO_x:H/ a-SiN_x:H on front surface of c-Si solar cells. As the refractive index of the

films are close to silicon, hence it also acts as an anti-reflection coating (ARC) to reduce optical losses in silicon solar cell.

Keywords: chemical Vapor deposition. Interface charge density, fixed charge density, passiva

References:

[1]. Armin G. Aberle, Prog. in Photovolt: Res. Appl. 2000; **8**; 473-487

THE EFFECT OF BRIDGING GROUP ON DIFFERENT LC PROPERTIES OF FLUORINATED LIQUID CRYSTALS

B. K. Singha[a], S. Haldar[a], P. K. Mandal[a]

[a]*Physics Department, North Bengal University, Darjeeling, India.*

(Research Area: Liquid Crystals)

Abstract: Five fluorinated nematic liquid crystals with dimethylene spacer have been investigated by Optical Polarizing Microscopy (OPM), Differential Scanning Calorimetry (DSC) and Dielectric Spectroscopy techniques. The effect of different structural elements such as linking group, rings and incorporation of fluorine atom is discussed. Structural changes cause to vary the liquid crystal parameters like dielectric anisotropy ($\Delta\epsilon$), dipole moment (μ), splay elastic constant (K_{11}) , activation energy (E_a) and relaxation time (τ) considerably. Broader nematic ranges are found in all investigated compounds with highest observed value $100^{O}C$ of Compound 1.Comparatively smaller value of K_{11} of the order of 10^{-11} is found in all cases thereby smaller value of switching time may be achieved using these compounds in display applications. Undesirable energy absorptions are found to restrict from few hundred kHz to MHz regime. Activation energy of thermally activated relaxations is found to be < 30 kJ/mol in all cases. Smaller value of threshold voltage is observed as a result of lower value in K_{11}. Smaller inclination of resultant dipole moment relative to para-axis causes higher value of axial dipole moment which is responsible of reducing V_{th} ,an important parameter in display applications.

Keywords: bridging group; dielectric spectroscopy; threshold voltage; dipole moment; splay elastic constant; activation energy.

ELECTRONIC STRUCTURES, MAGNETIC PROPERTIES AND STRAIN EFFECTS OF QUATERNARY HEUSLER ALLOYZrRuTiIn

R. B. Ray[1] and G. C. Kaphle[2]

[1]*Central Department of Physics, Tribhuvan University, Kirtipur, Kathmandu, Nepal*
[2]*Central Department of Physics, Tribhuvan University, Kirtipur, Kathmandu, Nepal*

(Research Area: Condensed Matter Physics)

Abstract: Using first-principles calculations, we investigate the electronic structure, magnetic properties andstrain effects of quaternary Heusler alloy ZrRuTiIn. Based on the density functional theory (DFT), theselfconsistent full-potential linearized-augmented plane-wave (FPLAPW) method with thegeneralized gradient approximation (GGA) was used to treat the exchange correlation energy for theentire calculations. During electronic structure calculations, GGA+U technique was utilized forstrongly correlated electrons of the compound. We used the values of U as 1 eV, 2 eV and 1.5 eV forthe elements Zr, Ru and Ti respectively. The estimated values of formation and cohesive energiesconfirms that the compound ZrRuTiIn is ermodynamically stable material according to theory. Thecalculated total spin magnetic moment of ZrRuTiIn is 1 μB and satisfying the well-known Slater-Pauling 19 electron rule, conforming the existence of the half-metallic gap. The calculated Curietemperature of the compound exceed the room temperature, making the compound promisingcandidate for spintronic applications. The GGA and mBJ calculation results imply that the compound

ZrRuTiIn is weak half-metallic in nature with considerable band gap of 0.419 eV and half-metallicband gap of 0.091 eV . Finally, the effects of uniform strain have been investigated and it is seen thatthe half-metallicity can be reduced, destroyed or enhanced by a uniform strain.

Keywords: Quaternary Heusler alloy, Density functional theory

References

[1] F. Dahmane et al., *Journal of Superconductivity and Novel Magnetism* **28**, 2063-2069 (2015).

[2] L. Feng et al., *Journal of Magnetism and Magnetic Material* **351**, 92-97 (2014).

[3] S. M. Azar et al., *Journal of Magnetism and Magnetic Material* **10,** 324 (2007).

FIRST PRINCIPLES STUDY OF ELECTRONIC AND THERMOELECTRIC PROPERTIES OF RHODIUM DOPED La FILLED SKUTTERUDITE

N. Limbu[1,2*], A. Saxena [1], A. Shankar [2]

[1]*Department of Physics, North-Eastern Hill University, Shillong, India-793022.*

[2]*Condensed Matter Theory Research Lab, Department of Physics, Kurseong, College, Darjeeling, West Bengal, India – 734203.*

(Research Area: Energy Materials)

Abstract: The electronic and thermoelectric properties of $LaOs_3RhSb_{12}$ have been investigated within the framework of the density functional theory using the full potential-linearized augmented plane wave (FP-LAPW) method. The calculated lattice constant (9.478 Å) corresponding to the minimum energy for the system is obtained. The energy band structure of the sample material suggests the semiconducting nature with an indirect energy gap of 0.24 eV along *N*-*Γ* diretion ofBrillouin Zone. The energy bands also reflects the parabolic and flat band like features. The positive magnitude of *S* over the whole temperature regionindicates that the majority of charge carrier is hole with the highest value of Seebeck coefficient for the sample alloy equal to 161 μV/K at 1000 K. The lattice thermal conductivity (K_L) of the sample alloy is found to reduce with increase in temperature. The semiconducting band structure along with high *S* and low value of K_L makes this alloy one of the potential candidate for the thermoelectric applications.

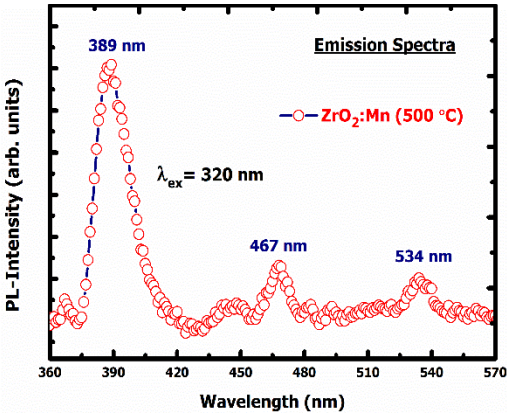
STRUCTURAL AND OPTICAL STUDIES OF Mn-DOPED ZrO_2 NANOCRYSTALS FOR WLEDs APPLICATIONS

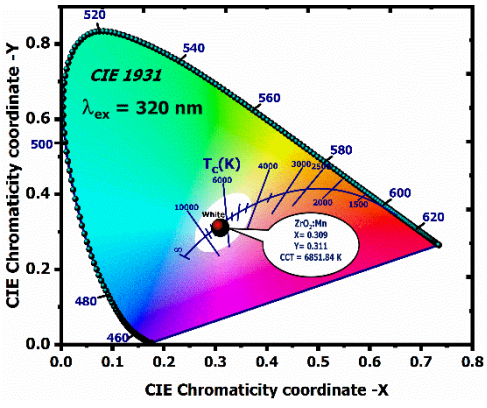
Laishram Robindro Singh and Sanjeeb Limbu

Department of Nanotechnology, North-Eastern Hill University, Shillong-793022, India

(Research Area: Nanomaterials)

Abstract: We report white-light emitting Mn-doped ZrO_2 nanocrystals (NCs) that are synthesized co-precipitation method. Tailoring three distinct emissions mechanism in these NCs, which are blue emissions at 389 and 476 nm respectively and Zn-defect state green emission at 534 nm, allowed us to achieve extinction wavelength tailorable white-light generation as studied fluorescence spectroscopy. These NCs will be promising as a single component white-light engines for solid-state lighting. The XRD pattern of pure and Mn doped ZrO2shows the formation of monoclinic and tetragonal phase of this nanocrystals. The energy gap of pure and Mn doped ZrO2 nanoparticles were computed by UV- Vis spectroscopy. The energy gap value of pure and Mn doped ZrO2 nanoparticles are found to be 2.02 and 5.07 eV, respectively. The CIE chromaticity coordinates diagram exhibits the formation of white color is located at white region of the color space. Which confirms these nanocrystals could be a potentials candidate for white LEDs fabrications.





Keywords: White-light emission, Doped Nanocrystals, Chromaticity, Fluorescence

References

[1] S. Rani, M. Kumar, S. Sharma, Catal Lett. **144**, 301 (2014)

[2] G. Bandekar, N.S. Rajurkar, I.S. Mulla, U.P. Mulik, D.P. Amalnerkar,

[3] P.V. Adhyapak, Appl Nanosci. **4**, 199 (2014)

[4] M. Hirano, C. Nakahara, K. Ota, O. Tanaike, M. Inagaki, J. SolidState Chem. **170**, 39 (2003)

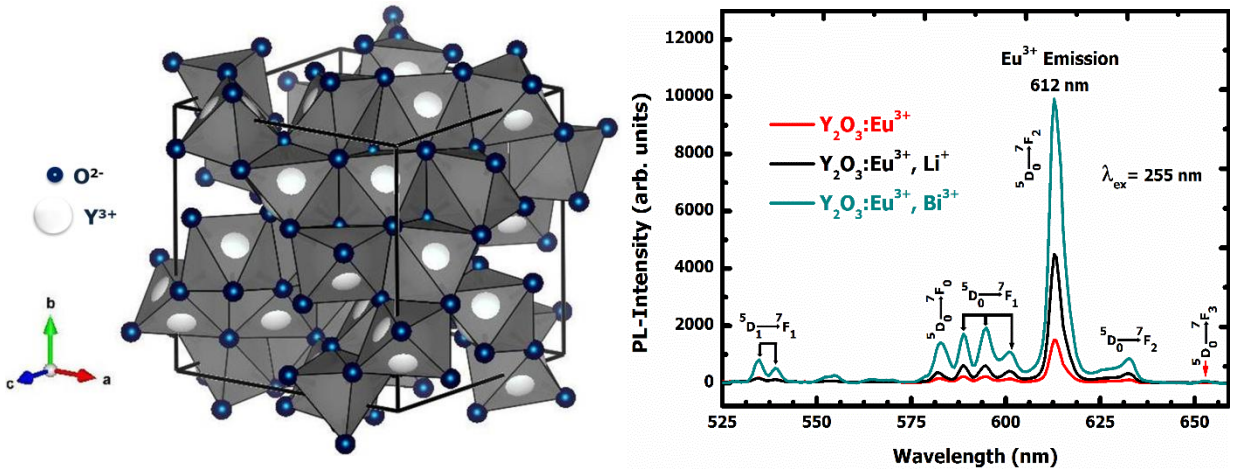
STRUCTURAL AND LUMINESCENCE STUDIES OF $Y_2O_3:Eu^{3+}$ NANOPHOSHORS SENSITIZED WITH Li^+/Bi^{3+} IONS FOR WLEDS APPLICATION

Sanjeeb Limbu and Laishram Robindro Singh

Department of Nanotechnology, North-Eastern Hill University, Shillong-793022, India

(Research Area: Nanomaterials)

Abstract. This work reports structural and luminescence properties of tunable $Y_2O_3:Eu^{3+}$ red-emitting nanophosphors sensitized with Li^+ and Bi^{3+} were prepared by wet chemical method. The structural property followed by X-ray diffraction analysis shows the nanophosphors have a body-centered cubic (I) phase with space group Ia-3 and point group symmetry m-3. No additional impurity peaks were observed within the range of the XRD pattern due to the Li^+ and Bi^{3+} ion. The unit cell structure of cubic Yttrium oxide (Y_2O_3) was modeled by using Rietveld refinement XRD data. The photoluminescence study shows the most intense red emission band at 612 nm due to the $^5D_0 \rightarrow {}^7F_2$ transition of Eu^{3+} ion in the C_{3i} and C_2 symmetry site of Y_2O_3 respectively. The emission band of Li^+ codoped $Y_2O_3:Eu^{3+}$ nanophosphor shows 2.97 times enhancement than the $Y_2O_3:Eu^{3+}$ one because of flux effect which is created by Li^+ ion. The Bi^{3+} codoped $Y_2O_3:Eu^{3+}$ nanophosphor shows the most intense band than the others that is due to the energy transfer from Bi^{3+} to Eu^{3+} ion. It shows 6.56 times higher enhancement than the emission band corresponds to $Y_2O_3:Eu^{3+}$ nanophosphor. The average lifetime was found to vary based on the different sensitizers used. The calculated Commission Internationale de l'Eclairage (CIE) 1931 chromaticity coordinates and correlated color temperature (CCT) values were tuned in the red region of the color space. All the results indicate that the prepared nanophosphor can be used as a potential red component to construct the white light for white light-emitting diodes fabrication.



Keywords: White light-emitting diode, Photoluminescence, Chromaticity, Nanophosphors

References

[1] M. I. Martinez-Rubio, T. G. Ireland, G. H. Fern, J. Silver and M. J. Snowden, *Langmuir*, 2001, 17, 7145-7149.

[2] W.-C. Chien, Y.-Y. Yu and C.-C. Yang, *Mater.Des.*, 2010, 31, 1737-1741.

[3] J. H. Zhang, Z. D. Hao, J. Li, X. Zhang, Y. Luo and G. Pan, *Light Sci. Appl.*, 2015, 4, 239-244.

[4] C. Liang, X. Huang and W. Huang, *J. Mater. Sci.: Mater.Electron.*, 2018, 29, 11271-11279.