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65th DAE SOLID STATE PHYSICS SYMPOSIUM

Dec 15 - 19, 2021

PROGRAMME & ABSTRACTS

Venue
DAE Convention Centre
Anushaktinagar, Mumbai

Organized by
Bhabha Atomic Research Centre
Mumbai

Sponsored by
Board of Research in Nuclear Sciences
Department of Atomic Energy
Government of India

65th DAE Solid State Physics Symposium

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Bhabha Atomic Research Centre, Mumbai

Programme and Abstracts

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Board of Research in Nuclear Sciences
Department of Atomic Energy
Government of India

के. एन. व्यास
K. N. Vyas

सत्यमेव जयते
भारत सरकार
Government of India

अध्यक्ष, परमाणु ऊर्जा आयोग
व
सचिव, परमाणु ऊर्जा विभाग
Chairman, Atomic Energy Commission
&
Secretary, Department of Atomic Energy

MESSAGE

It is a pleasure to note that the DAE Solid State Physics Symposium (DAE-SSPS) is being organized at Bhabha Atomic Research Centre, Mumbai during December 15 - 19, 2021. This flagship symposium of the Department of Atomic Energy is the 65th in the series and has traditionally been a well-attended symposium with a prestige of its own. The symposium has been playing an important role in promoting and encouraging research in the domain of condensed matter physics. The event is fully sponsored by Board of Research in Nuclear Sciences (BRNS), DAE with researchers from all over the country looking forward to participate in it. This year, nearly 1000 participants will be attending the event being conducted in a hybrid a mode.

The scientific deliberations in the form of invited talks, contributory papers, and the presentations by Young Achiever Award nominees and of PhD scholars would surely be an enriching experience for all the participants. The presence of distinguished invitees and enthusiastic young scientists would definitely lead to significant exchange of knowledge and ideas in the field.

I wish all the delegates a very fruitful and stimulating scientific interactions and a great success to this event.

(K. N. Vyas)

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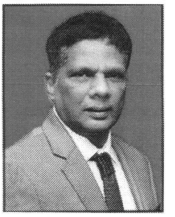
डॉ. अजित कुमार मोहान्ती
Dr. Ajit Kumar Mohanty

सत्यमेव जयते
भारत सरकार
Government of India

निदेशक, भाभा परमाणु अनुसंधान केंद्र
Director, Bhabha Atomic Research Centre
सदस्य, परमाणु ऊर्जा आयोग
Member, Atomic Energy Commission



MESSAGE

I am glad to note that the 65thDAE Solid State Physics Symposium (DAE-SSPS) is being held at Bhabha Atomic Research Centre, Mumbai during December 15 - 19, 2021. This very prestigious and popular series of symposia has been organised by BARC annually in various parts of the country and is one of the largest symposium attended by delegates from all DAE units, universities, national institutes and laboratories.

DAE-SSPS has a reputation of providing a very interactive forum for scientific discussions amongst scientists, engineers and researchers in important and emerging topics of condensed matter physics including magnetism, quantum phenomena, thin films, strongly correlated materials, nano-photonics, matter under extreme conditions and energy materials. A large number of nearly 1000 manuscripts received this year under the various categories is a testimony to the interest and popularity of this flagship symposium. The young achiever and PhD thesis awards category also have an overwhelming response indicating the high value attached to them by the scientific community in the field. I am sure that DAE-SSPS 2021 will meet the expectations for the desired objectives of scintillating scientific deliberations and generation of new research ideas.

I convey my best wishes for all round success of the symposium.

Ajit Kumar Mohanty
(Ajit Kumar Mohanty)

Dr. S.M. Yusuf, D.Sc (Hon), FASc, FNASc
डॉ. एस. एम. युसुफ
Director, Physics Group
निदेशक, भौतिकी वर्ग

सत्यमेव जयते

भारतसरकार
GOVERNMENT OF INDIA
भाभा परमाणु अनुसंधान केंद्र
BHABHA ATOMIC RESEARCH CENTRE
भौतिकी वर्ग
PHYSICS GROUP
Mumbai 400085

राष्ट्र की सेवा में परमाणु
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भाभा परमाणु अनुसंधान केंद्र
BHABHA ATOMIC RESEARCH CENTRE

Message

It is our great pleasure to organize the 65th DAE Solid State Physics Symposium (DAE SSPS 2021). It is indeed a matter of pride and privilege that the Physics Group of Bhabha Atomic Research Centre has been organizing this flagship symposium of the Department every year. This symposium is being held since 1957 in different parts of the country in various universities and research institutions. It remains the largest attended symposium in solid state and condensed matter physics in the country despite the fact that several smaller meetings are held on various specialized topics. Over the years, the popularity of this symposium has grown enormously. This year, the symposium is being held at the DAE Convention centre, Anushaktinagar, Mumbai during December 15-19 2021.

DAE SSPS has been providing an excellent forum for close and fruitful scientific interactions among researchers in several important and emerging areas of condensed matter physics. These include quantum phenomena, superconductivity, magnetism, soft condensed matter, spintronics, semiconductors, nano materials, glasses, amorphous & composite systems, thin films, multi-layered structures, crystals, energy materials, *etc*. The tradition of giving Young Achiever and the Best Thesis Awards in this symposium has encouraged healthy competition among young researchers in condensed matter physics. It has become one of the attractive aspects of this event, which young researchers look forward to participate and compete.

My colleagues from Physics Group, BARC have put in commendable efforts for organising this symposium with an excellent scientific program.

I extend my warm greetings to all the distinguished delegates and participants. I look forward to fruitful and exciting scientific deliberations in the DAE SSPS2021.

Md. Yusuf

(S. M. Yusuf)

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भारत सरकार
Government of India
भाभा परमाणु अनुसंधान केन्द्र
Bhabha Atomic Research Centre

भाभा परमाणु अनुसंधान केंद्र
BHABHA ATOMIC RESEARCH CENTRE

डॉ. दिनेश वी. उडुपा
Dr. Dinesh V. Udupa
अध्यक्ष,
परमाणु एवं आणविक भौतिकी प्रभाग
Head,
Atomic & Molecular Physics Division

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दूरभाष: ०२२-२५५९३८७१
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Message from Convener

It is indeed a matter of privilege and a great pleasure to organise the prestigious event of the DAE Solid State Physics Symposium. The symposium is the 65th in the series this year, and is organised at DAE Convention Centre Anushaktinagar Mumbai during December 15-19, 2021. The event is in a hybrid mode, keeping up to the requirement of the times, where only local participants will be present at the venue physically whereas others will attend using the on-line platform.

DAE SSPS has been traditionally covering all the important and emerging areas in condensed matter physics. This year the themes include Quantum Phenomena, Magnetism, Superconductivity, Strongly correlated Materials, Nano-photonics, Surfaces & Thin Films, Energy Materials, Matter under extreme conditions, Condensed Matter Theory, Chemical Physics and Experimental Techniques. This year we have received nearly 1000 papers, out of which 741 manuscripts were accepted for the presentation after they were reviewed by nearly 300 referees form all over the country. The technical sessions include plenary talks, invited talks, contributory oral presentations, PhD thesis and presentations by Young achiever award nominees.

I must acknowledge the efforts of the scientific secretaries, the Late Dr. C. L. Prajapat, Dr. Arup Biswas and Dr. Ajay Mishra in formulating an excellent program by their sincere hard work. They have played a commendable role in overcoming new challenges resulting from the hybrid mode of the conference, which is a new experience to all of us.

I extend my warm greetings to all the delegates and wish for a great success in having a fruitful and beneficial scientific deliberations in the symposium.

(Dinesh V. Udupa)

Advisory Committee

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Veerendra K. Sharma	BARC	Mumbai

SUBJECT CATEGORIES

a. Phase transitions and dynamics

b. Soft condensed matter includingbiological systems

c. Nano-materials

d. Experimental techniques and devices

e. Glasses and amorphous systems

f. Surfaces, interfaces, and thin films

g. Computational methods, and electronicstructures

h. Single crystals growth and characterization

i. Transport properties

j. Semiconductor physics

k. Magnetism, superconductivity, and spintronics

l. Energy materials

m. 1-D and 2-D

AWARD CATEGORIES

TH: Ph. D thesis Award

YAA: Young Achiever Award

Best Poster Award

Program Overview

Day 1: Wednesday, December 15, 2021

08:00-09.30	**Registration** **(*Venue: Reception area of DAE Convention Centre*)**
09.30-10:15	**Inaugural Function** **(*Venue: Auditorium 1*)**
10:15-11.00	**Plenary Talk** **PL-01: Amlan J. Pal *(UGC-DAE CSR, Indore)*** *Bandgap of Disordered Semiconductors in relation to Optoelectronic Devices*
11:00-11:30	**High Tea**
11:30-13:00	**Plenary Talks** **PL-02: Peter Fischer *(Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley CA, USA)*** *Advanced magnetic x-ray spectro-microscopies of novel topological spin textures* **PL-03: Douglas S. Galvao *(State University of Campinas and Brazilian Academy of Sciences, Brasil)*** *Multi-scale Modeling of Nanomaterials: From Nanotubes to Ants*
13:00-14:00	**Lunch Break**
14:00-16:00	**Quantum Phenomenon** **(*Venue: Auditorium 1*)**
	IT-01: Pinaki Majumdar *(HRI, Prayagraj, UP, India)* *The Langevin approach to nonequilibrium correlated electron systems* **IT-02: Bahadur Singh (*TIFR, Mumbai, India*)** *Topological quantum magnets: From concept to material realizations* **IT-03: Anup Kumar Bera *(Bhabha Atomic Research Centre, Mumbai)*** *Experimental Realization of Quantum Phenomena in 1D Antiferromagnets* **IT-04: Rajib Batabyal *(UGC-DAE CSR, Indore)***

	Topological Weyl Fermions Measured on the Surfaces
14:00-16:00	**Condensed Matter Theory** ***(Venue: Auditorium 2)***
	IT-05: Shobhana Narasimhan (*JNCASR, Bangaluru, India*) *Diffusion and Sintering of Ultrasmall Nanoparticles: Mechanisms & Scaling Relations* **IT-06: Brijesh Kumar *(JNU, New Delhi, India)*** *Inversion and Quantum Oscillations in Kondo insulators* **IT-07: Rajamani Raghunathan *(UGC-DAE, CSR, Indore)*** *Theoretical modeling of charge-disproportionation in BaBiO3* **IT-08: David J. Singh *(University of Missouri, Columbia, USA)*** *Electronic and Phononic Features for High Thermoelectric Performance*
16:00-16:30	**Tea and Poster Presentation**
16:00-18:00	**Poster Presentation: Contributory Paper** **(*Venue: www.daessps.in*)**
	16:00-17.00: a0001 to a0011, b0001 to b0009, c0001 to c0018, d0002 to d0010, e0003 to e0007, f0002 to f0013, g0001 to g0010, k0001 to k0010, l0002 to l0013 **17:00-18:00:** c0019 to c0035, f0014 to f0025, g0011 to g0018, h0002 to h0007, i0001 to i0010, j0003 to j0008 k0011 to k0024, l0014 to l0026, m0001 to m0008
16:00-18:00	**Poster Presentation: YAA** (***Venue: Auditorium 1***)
	y0002 to y0014
	Poster Presentation: YAA (***Venue: Auditorium 2***)
	y0016 to y0036

Day 2: Thursday, December 16, 2021

09:30-11:00	**Superconductivity** ***(Venue: Auditorium 1)***
	IT-09: S. Patnaik ***(Jawaharlal Nehru University, New Delhi, India)*** *Signatures of Topological Superconductivity in Sr intercalated Bi2Se3* **IT-10: Girish Sharma** ***(Indian Institute of Technology, Mandi, India)*** *Superconductivity and metallic state transport in magic angle twisted bilayer graphenes* **Contributed Oral Presentation:** *a0006 and k0010*
09:30-11:00	**Physics Using Neutron and Synchrotron** ***(Venue: Auditorium 2)***
	IT-11: Debasis Sen ***(Bhabha Atomic Research Centre, Mumbai, India)*** *Elucidating the integrity during crisis in colloidal & emulsion droplets by SANS and SAXS* **IT-12: S. K. Rai** ***(RRCAT, Indore, India)*** *A Versatile X-ray Scattering and Diffraction Beamline for Engineering Applications at Indus-2 Synchrotron Source* **Contributed Oral Presentation:** *e0024 and l0014*
11:00-11:30	**Tea Break**
11:30-13:00	**Contributed Oral Presentation** ***(Venue: Auditorium 1)***
	b0014, b0020, c0016, c0035, c0045, j0018
11:30-13:00	**Contributed Oral Presentation** ***(Venue: Auditorium 2)***
	e0004, f0024, f0043, f0091, g0005, g0006
13:00-14:00	**Lunch Break**

14:00-16:00	**Magnetism** ***(Venue: Auditorium 1)***
	IT-13: Anamitra Mukherjee ***(NI SER, HBNI, Jatni, India)*** *Creating tunable finite temperature half-metal out of an antiferromagnetic Mott insulator* **IT-14: Basavaraj Angadi** ***(Bangalore University, Bangalore, India)*** *Multiferroic properties of Pb based perovskites* **IT-15: Nirmalya Ballav** ***(IISER, Pune, India)*** *Anchoring Cu(II)-Based S=1/2 Kagome Lattices on Functionalized Graphene* **Contributed Oral Presentation:** *k0094 and k0106*
14:00-16:00	**Chemical Physics** ***(Venue: Auditorium 2)***
	IT-16: Brendan J. Kennedy ***(The University of Sydney, Sydney NSW Australia)*** *Phase Transitions and Disorder: A Tale of Two Scheelites* **IT-17: P. A. Hassan** ***(BARC, Mumbai, India)*** *Jammed micelles in water-free supercooled matrix: Evidence from small angle scattering* **IT-18: Deepak Chopra** ***(IISER, Bhopal)*** *Exploring the Role of Crystal Chemistry in Materials Science* **IT-19: Ajit K. Mahapatro (*University of Delhi, Delhi, India*)** *Nanostructured calcium cobalt oxide with enhanced properties for thermoelectric generation*
16:00-16:30	**Tea Break and Poster Presentation**
16:00-18:00	**Poster Presentation: Contributory Paper** **(*Venue: www.daessps.in*)**
	16.00-17.00: a0012 to a0019, b0010 to b0015, c0036 to c0051, d0011 to d0018, e008 to e0014, f0026 to f0033, g0019 to g0028, k0025 to k0037, l0027 to l0042

	17.00-18.00: c0052 to c0067, f0034 to f0043, g0029 to g0037, h0008 to h0013, i0011 to i0020, j0010 to j0014, k0038 to k0047, l0043 to l0054, m0010 to m0017
16:00-18:00	**Poster Presentation: Ph.D Thesis** (***Venue: Auditorium 1***)
	t0005 to t0028
	Poster Presentation: Ph.D Thesis ***(Venue: Auditorium 2)***
	t0029 to t0057

Day 3: Friday, December 17, 2021

09:30-11:00	**Experimental Techniques** ***(Venue: Auditorium 1)***
	IT-20: D. Banerjee ***(VECC, Kolkata, India)*** *Time Differential Perturbed Angular Correlation Spectroscopy: A Potential Tool to probe Materials Structure in Atomic Scale* **IT-21: K. Prabakar** ***(IGCAR, Kalpakkam, India)*** *Microcantilevers for Ultrafast Humidity and Ultrasensitive Temperature Sensing Applications* **Contributed Oral Presentation:** *d0007 and d0046*
09:30-11:00	**Young Achiever Award Presentation** ***(Venue: Auditorium 2)***
11:00-11:30	**Tea Break**
11:30-13:00	**Contributed Oral Presentation** ***(Venue: Auditorium 1)***
	g0028, h0002, h0033, i0024, i0032, j0016
11:30-13:00	**Young Achiever Award Presentation-Continued** ***(Venue: Auditorium 2)***
13:00-14:00	**Lunch Break**
14:00-16:00	**Strongly Correlated Materials** ***(Venue: Auditorium 1)***
	IT-22: N S Vidhydhiraja ***(J. N. C. A. S. R. Bengaluru, India)*** *Emergent non-Fermi liquid behaviour in disordered, strongly interacting systems* **IT-23: Subhro Bhattacharjee** ***(International centre for theoretical sciences, Tata Institute of Fundamental Research Bengaluru, India)*** *Spin-orbit coupled Dirac Fermions*

	IT-24: S. Thirupathaiah ***(S. N. Bose National Centre for Basic Sciences, Kolkata, India)*** *Strong Electronic Correlations Observed in Colossal Thermoelectric Material K0.65RhO2 Using Angle-Resolved Photoelectron Spectroscopy (ARPES)* **IT-25: Chandrasekhar Murapaka** ***(Indian Institute of Technology, Hyderabad, India)*** *Spin-orbitronics: Interconversion between charge and spin currents*
14:00-16:00	***Glass, Alloy and Composite Systems*** ***(Venue: Auditorium 2)***
	IT-26: K. R. Priolkar (*Goa university, Goa, India*) *Defect induced Non-ergodic Ground States in Martensites* **IT-27: Kinshuk Dasgupta** ***(Bhabha Atomic Research Centre, Mumbai, India)*** *Tailoring the properties of composites with carbon nanomaterials as reinforcement* **IT-28: S. Abhaya (*IGCAR Kalpakkam, India*)** *Positron beam studies on the Irradiation damage resistance in High entropy alloys* **IT-29: S. Chatterjee** ***(UGC-DAE CSR, Kolkata, India)*** *Doping site induced modification of the magnetic structure of MnNiGe alloys*
16:00-16:30	**Tea Break and Poster Presentation**
16:00-18:00	**Poster Presentation: Contributory Paper** ***(Venue: www.daessps.in)***
	16:00-17:00: a0020 to a0027, b0017 to b0023, c0068 to c0085, d0019 to d0025, e0015 to e0024, f0044 to f0052, g0038 to g0046, k0050 to k0061, l0055 to l0067 **17:00-18:00:** c0086 to c0102, f0053 to f0063, g0047 to g0056, h0014 to h0020, i0021 to i0026, j0016 to j0021, k0062 to k0076, l0072 to l0084, m0018 to m0024

Day 4: Saturday, December 18, 2021

	Matter Under Extreme Conditions ***(Venue: Auditorium 1)***
09:30-11:00	**IT-30: Boby Joseph (*Elettra Sincrotrone-Trieste, Italy*)** *Pressure tuning of material properties: selected examples from the joint Indo-Italian beamline "Xpress" at Elettra–Synchrotron Trieste* **IT-31: Ranjan Mittal *(BARC, Mumbai, India)*** *Thermodynamic Behaviour of Graphite Under Extreme Conditions of Nuclear Radiation, Pressure and Temperature* **IT-32: K. K. Pandey (*BARC, Mumbai, India*)** *Recent advances in the study of plastic strain induced phase transitions under high pressures*
09:30-11:00	**Best Thesis Presentation** ***(Venue: Auditorium 2)***
11:00-11:30	**Tea Break**
11:30-13:00	**Contributed Oral Presentation** ***(Venue: Auditorium 1)***
	a0016, k0091, l0024, l0047, m0008, m0012
11:30-13:00	**Best Thesis Presentation Continued** ***(Venue: Auditorium 2)***
13:00-14:00	**Lunch Break**
14:00-16:00	**Nano-Photonics** ***(Venue: Auditorium 1)***
	IT-33: Sushil Mujumdar *(TIFR, Mumbai, India)* *Experimental evidence of a novel anomalous transport regime in hybrid, non-Hermitian disordered systems* **IT-34: Saikat Ghosh (*IIT, Kanpur, U.P., India*)** *Graphene drum resonators coupled over long distances: towards controlled phononic time crystals*

	IT-35: Jitendra Nath Roy ***(Nazrul University, Asanso, West Bengal, India)*** *Organic Photodetector As Next Generation Light Detection: Challenges And Opportunities* **IT-36: Mrinal Pal (*CSIR-Central Glass and Ceramic Research Institute, Kolkata, India*)** *Defect mediated multicolored emission from pristine ZnO nanostructure: A voyage towards single source white LED*
14:00-16:00	**Surface, Thin Films and Interfaces** ***(Venue: Auditorium 2)***
	IT-37: Sanjay K. Srivastava (*NPL, New Delhi, India*) *Surface Micro Engineering of Silicon for Efficient and Cost Effective PEDOT:PSS/Silicon Hybrid Solar Cells* **IT-38: R. J. Choudhary** ***(UGC DAE, CSR, Indore)*** *Probing Magnetic Properties of Oxides Thin Films Using XMCD Studies at Indus-2 Synchrotron Source* **IT-39: Suvankar Chakraverty** ***(INST, Mohali, India)*** *Unique Magnetotransport in $KTaO_3$ based conducting interfaces: Planar Hall effect, Anomalus Hall effect, Shubnikov-de Haas oscillations, Berry's phase, Chiral Anomaly(?)* **IT-40: Satyaprakash Sahoo** ***(Institute of Physics, Bhubaneswar)*** *Engineering van der Waals solids for tunable optical and electronic properties*
16:00-16:30	**Tea Break and Poster Presentation**
16:00-18:00	**Poster Presentation: Contributory Paper** ***(Venue: www.daessps.in)***
	16:00-17:00: a0028 to a0035, b0024 to b0034, c0103 to c0118, d0026 to d0036, e0025 to e0029, f0064 to f0072, g0057 to g0064, k0077 to k0087, l0086 to l0102 **17:00-18:00:** c0119 to c0136, f0078 to f0088, g0065 to g0073, h0021 to h0027, i0027 to i0032, j0022 to j0026, k0088 to k0099, l0103 to l0113, m0025 to m0031

Day 5: Sunday, December 19, 2021

09:30-11:00	**Energy Materials** ***(Venue: Auditorium 1)***
	IT-41: Balaji P Mandal ***(BARC, Mumbai, India)*** *Lithium based Battery: Fundamentals and Challenges Ahead* **IT-42: Madhu Chennabasappa (*Siddaganga Institute of Technology, Tumkur, Karnataka, India*)** *Surface modification by metal-oxide nanoparticle coatings for improving the cycling characteristics of the cathode material* **IT-43: Utpal Sarkar** ***(Assam University, Silchar, India)*** *Designing of Carbon Based Energy Material*
11:00-11:30	**Tea Break**
11:30-13:15	**Poster Presentation: Contributory Paper** ***(Venue: www.daessps.in)***
	11:30-12:30: a0036 to a0043, b0036 to b0041, c0138 to c0152, d0039 to d0046, e0030 to e0033, f0089 to f0096, g0074 to g0082 **12:15-13:15:** h0028 to h0034, i0033 to i0041, j0027 to j0032, k0100 to k0107, l0115 to l0124, m0032 to m0036
13:15-14:00	**Lunch Break**
14:00-15:30	**Award Presentations and Concluding Session** ***(Venue: Auditorium 1)***

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Contributory Paper

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ABSTRACTS

PLENARY TALKS

PL-01

Bandgap of Disordered Semiconductors in relation to Optoelectronic Devices

Amlan J. Pal[1,2]
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[2]*School of Physical Sciences Indian Association for the Cultivation of ScienceJadavpur, Kolkata*
Email: director@csr.res.in

Disordered semiconductors have attracted significant attention for basic studies in physics as well as in a range of optoelectronic applications. Device physics in such applications, in principle, depended on light-matter interactions in which the optical bandgap and transport gap of the semiconductors play a primary role. Hence, appropriate tuning of the bandgap in disordered semiconductors remained important in optimizing the device performance.

In many disordered semiconductors, the relationship between composition and functional properties, such as optical bandgap, often exhibits a quadratic behavior giving rise to a phenomenon, called “bandgap bowing”. The underlying mechanism of this ‘bow-like' evolution of bandgap in some oxides, chalcogenides, and of late halide perovskites is yet to be understood. To know the origin of bandgap bowing, we have probed the conduction and valence band-edges (CB and VB) of some alloyed semiconductors to inquire about the band responsible for yielding the bowing.

In such semiconductors, the presence of a significant density of defect states within the bandgap results in sub-bandgap absorbance in the absorption spectrum (Urbach tailing). While optical absorption spectroscopy provides a ‘macroscopic’ insight into the phenomenon, the contribution of individual band-edges is needed to be identified on a ‘microscopic’ scale. We have obtained accurate information on the band-edges leading to a precise quantification of Urbach energy in disordered semiconductors.

To optimize the performance of optoelectronic devices, it is a prerequisite to visualize the band-diagram of the active layers with respect to the electrodes as ‘seen’ by charge carriers. In this regard, we have employed scanning tunneling spectroscopy (STS) to probe the energy levels of a range of semiconductors upon varied formation conditions. STS probed the density of states (DOS) of the semiconductors and thereby CB and VB, separately, with respect to the Fermi energy (E_F). Such information when combined with the E_F obtained from Kelvin probe force microscopy (KPFM) studies can provide the complete energy landscape of a semiconductor and also of heterojunction devices.

Pl-02

Advanced magnetic x-ray spectro-microscopies of novel topological spin textures

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Spin textures and their dynamics hold the key to understand and control the properties, behavior and functionalities of novel magnetic materials, which can impact the speed, size and energy efficiency of spin driven technologies. Topology, frustration, and bespoke geometries that impact spin textures have recently attracted significant scientific interest and led to intense research addressing a broad spectrum of challenging scientific and technological questions, including stability, dynamics, nucleation, and transport in novel spin textures, such as chiral bobbers, magnetic hopfions and torons,skyrmion tubes, and curvilinear magnetism [1].

Advanced characterization tools that provide magnetic sensitivity to spin textures, disentangling the role of individual components in heterogeneous material at high spatial resolution, ultimately at buried interfaces and in all three dimensions [2], and at high temporal resolution to capture the spin dynamics across scales, are required to address those questions, and are therefore of large scientific interest.

Various magnetic soft X-ray spectro-microscopies [3] using polarized soft x-rays provide unique characterization opportunities to study the statics and dynamics of spin textures in magnetic materials combining X-ray magnetic circular dichroism (X-MCD) as element specific, quantifiable magnetic contrast mechanism with spatial and temporal resolutions down to fundamental magnetic length, time, and energy scales.

Current developments of x-ray sources aim to increase dramatically the coherence of x-rays opening the path to new techniques, such as ptychography [4] or x-ray photo-correlation spectroscopy (XPCS) [5] that allow unprecedented studies of nanoscale heterogeneity, complexity, and fluctuations.

I will review recent achievements and future opportunities with magnetic x-ray spectro-microscopies. Examples will address static properties and dynamic behavior of various magnetic skyrmion [6,7] and Hopfion [8] textures with potential application to novel magnetic logic and storage devices, and will include results from an XPCS study at LCLS with a novel 2-pulse scheme that allowed to discover an unexpected and drastic change of the correlation times in nanoscale spin fluctuations near phase boundaries, i.e., in the skyrmion phase, and near the boundary with the stripe phase of a multilayered Fe/Gd system [5].

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PL-03

Multi-scale Modeling of Nanomaterials: From Nanotubes to Ants

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The sp, sp2, sp3 carbon hybridizations allow an almost infinite number of different structures with tunable mechanical and electronic properties. These structures can exhibit different topologies with different electronic dimensions (0-fullerenes,1-nanotubes, 2-graphene, 3-diamond).These topologies can be exploited to create a large class of different materials, such as buckypapers [1], carbon nanotube-based artificial muscles [2,3], foams [4], auxetic crystals [5], etc. These materials present extremely complex morphologies, which results in a difficult challenge to realistically model their mechanical and structural properties. In this talk, we will present and discuss multi-scale (from nano to macro scale) approaches to model these materials, including the use of bioinspired artificial intelligence methods (such as the bioinspired ANT algorithms). Of particular interest are the new molecular dynamics simulations techniques based on reactive potentials that allow handling multi-million atom systems. These techniques can be also used for non-carbon materials, such as chalcogenides [6] and non-van der Waals solids [7].

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INVITED TALKS

IT-01

The Langevin approach to nonequilibrium correlatedelectron systems

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The Langevin equation has been a major tool for studying dynamicsin classical stochastic systems. It can probe equilibrium fluctuations,the approach to equilibrium, and even driven systems. While itsorigin lies in probing "single particle" motion it is frequently used in extended, or many particle, systems. Can this approach be of help inunderstanding the thermal physics of correlated quantum systems? Iwill outline the approach, and discuss examples from electron-electronand electron-phonon systems, both in and out of equilibrium.

IT-02

Topological quantum magnets: From concept to materials realizations

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The realization of topological materials which exhibit exotic, disorder-resistant states has opened a new realm ofmaterials research not only for their potential for exploring fundamental physics questions but also for the opportunities they offer for sparking the next technological revolution. I will discuss how the interplay of wavefunction topology, crystalline symmetries, and quantum interactions generate exotic topological phases that can be manipulated through external controls of electric/magnetic fields, strains, pressure, and photo- or chemical doping. I will highlight some of our recent breakthroughs aimed at the prediction of topological quantum magnets that can support unconventional topological states at the charge neutrality point with anomalous transport properties.

IT-03

Experimental Realization of Quantum Phenomenain 1D Antiferromagnets

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The field of low-dimensional quantum magnetism started a century ago during the early development of quantum mechanics. ErnstIsing,in 1925,derived an exact solution of the one dimensional (1D) spin-chain (having a preferred direction) with nearest neighbor interaction only [1]. Followed by, Bethe introduced his famous “ansatz” method in 1931 to find the exact quantum ground state of the antiferromagnetic Heisenberg model in 1D [2].The ground states of 1D uniform S = 1/2 chains are different in the Ising and Heisenberg models. While the chain becomes ordered at zero temperature in the Ising limit, it remains disordered even at zero-temperature in the Heisenberg limit. Further, Haldane in 1983 shown that the integer and half-integeruniform Heisenberg spin-chains are fundamentally different [3]. The spin-1/2 chain has gapless excitations—spinonscarrying fractionalized spin S = 1/2. On the other hand, the uniform spin-1 chain has gapped excitations where nonmagnetic spin singlet ground state is well separated in energy from the first excited states of spin-triplets (magnons carrying spin S = 1).

However, the experimental realization/verification of the basic theory of low-dimensional (low-D) magnetism, as advanced by Ising,Heisenberg and Bethe,begins much laterin the last decade of the 20th century. Over last two decades, the advancement of solid state chemistry to synthesis model low dimensional spin-systems, as well as the advancement of experimental facilities, especially neutron scatterings, with dedicated sample environments

allow to explore and realize various quantum phenomena in low dimensional spin systems mainly based on complex transition metal oxides.

In this talk, I will present our experimental results (especially by using neutron scatterings technique) of the naturally grown quasi-1D spin-chain antiferromagnets SrM2V2O8 (M = Ni and Co) [4-13]. The results provide experimental realization of several quantum phenomena of the 1D antiferromagnets, including—topologically protected Haldane state, field-induced quantum phase transition, condensed matter analogue of the quark-confinement, quantum criticality, and the Bethe-string states.

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IT-04

Topological Weyl Fermions Measured on the Surfaces

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Existence of topological “Fermi-arc” surface states is guaranteed by the bulk Weyl nodes and appears as a consequence of bulk-boundary correspondence in Weyl semimetals. Bulk Weyl nodes are formed when non-degenerate band touches each other under broken inversion or time reversal symmetry. We carried out scanning tunneling spectroscopy (STS) experiments to visualize the topological surface Fermi arcs in both the inversion and time reversal symmetry broken Weyl semimetals e.g. TaAs and Co3Sn2S2 respectively and verify their classifications. In inversion symmetry broken TaAs, we find high level of topological protection of the surface Fermi arcs against the surface potential through its structure of the plane-wave like Bloch wave function in the Brillouin zone (BZ). On the other hand, in time reversal symmetry broken Co3Sn2S2, we find the topological Fermi arcs are highly susceptible to the surface potential that changes its connectivity in the BZ on different surface terminations and the dispersion of the arcs. This allows to manipulate these topological arcs through the surface potential.

IT-05

Diffusion and Sintering of Ultrasmall Nanoparticles: Mechanisms & Scaling Relations

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Small nanoparticles supported on substrates are of technological interest because they can be excellent catalysts for many industrially and environmentally important reactions. They can also possess interesting physical properties, e.g., small particles of some elements can be

nanomagnets, even if the corresponding bulk material is non-magnetic. Properties of interest, such as chemical reactivity and magnetic moments, are highly size-sensitive -- typically, the catalytic activity of metal nanoparticles increases sharply as the size is decreased. However, nanoparticles are intrinsically unstable with respect to sintering: it is always energetically favorable for two or more nanoparticles to coalesce to form a larger-sized particle. This process is one of the important causes of nanocatalyst degradation. It is therefore of interest to study the processes by which nanoparticles diffuse on substrates, and fuse together.

I will present work in our group on the diffusion and sintering of ultrasmall small noble metal particles on a MgO support. We find that these clusters diffuse by unexpectedly complex motions that do not correspond to simple translations. The diffusion mechanism depends upon both the atomic species and the number of atoms in the nanoparticle. We find unexpected scaling relations between diffusion barriers and other quantities (such as the melting temperature of the bulk metal), we will discuss the origin and implications of such scaling relations.

IT-06

Inversion and Quantum Oscillations in Kondo insulators

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The quantum oscillations observed in Kondo insulators pose a challenge to the common knowledge that the de Haas-van Alphen effect occurs only in metals. In this talk, we will present our understanding of this problem in terms of an original theory of Kondo insulators [1,2], formulated using a novel representation of electrons [3]. Through this theory, we have discovered the inversion exhibited by the gapped charged quasiparticles in Kondo insulators, and found this inversion to determine whether or not the quantum oscillations would occur in the insulating bulk.

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IT-07

Theoretical modeling of charge-disproportionation in $BaBiO_3$

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Nature and mechanism of charge ordering (CO) in $BaBiO_3$ (BBO) has been debated for past several yearsbetween complete CO (Bi^{3+}-Bi^{5+}), oxygen 2p - 2p fluctuation in the negative delta regime and incomplete CO *a.k.a.* charge-disproportionation (CD) ($Bi^{4-\delta}$ - $Bi^{4+\delta}$) ($0<\delta<1$) [1-3]. Here, we present a new mechanism for CD using a molecular orbital (MO) approach [4]. We show that CD in BBO is governed by the dynamic fluctuation between Bi 6sp – O 2p hybridization that favours Bi^{5+}charge state and Bi 6p – O 2p hybridization that favours Bi^{3+} charge state, driven by the octahedral breathing mode. The model is further validated with results from density functional theory calculations using hybrid functional, HSE06. We also employ strain as an external perturbation to tune the CD and further show that CD can also be asymmetric ($Bi^{4-\delta 1}$ - $Bi^{4+\delta 2}$) ($0< |\delta 1| \text{and} |\delta 2|<1$). Results from x-ray spectroscopic studies also demonstrate the dynamic nature of CD that becomes quasi-static at room temperature in strained thin films and thus endorses our proposed model.

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IT-08

Electronic and Phononic Features for High Thermoelectric Performance

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The thermoelectric figure of merit, *ZT*, is a combination of thermal and electrical transport quantities that is strongly contraindicated in the sense that the particular combination of high electrical conductivity, high thermopower and low thermal conductivity does not naturally occur in textbook models. This talk discusses electronic and lattice dynamical features that resolve these contradictions in half-Heuslers and other materials thus providing ways of designing and discovering new themoelectrics.

IT-09

Signatures of Topological Superconductivity in Sr intercalated Bi_2Se_3

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The discovery of Dirac and Weyl semimetals has brought forth the condensed matter realization of Dirac/Weyl fermions, which were previously theorized as low energy excitations in high energy particle physics. In the recent past we have witnessed some exceptional developments in chalcogenide and pnictide materials that have been identified with such properties. Superconductivity derived from such exotic systems promises to usher-in new understanding of correlated electronic systems. In this talk we shall review electromagnetic properties of topological superconductor Sr-intercalated Bi_2Se_3 and study its pairing mechanism by muon spin rotation measurements. Furthermore, several transition metal mono-pnictides are under intense investigation for understanding properties of inversion-symmetry broken Weyl semimetals. Non-trivial Berry phase and chirality are important markers for characterizing topological measures of Weyl semimetals. We shall also discuss aspects of exceptional magneto-resistance seen in the normal state of these topological semimetals.

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IT-10

Superconductivity and metallic state transport in magic angle twisted bilayer graphenes

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We discuss our proposal of a purely electronic mechanism for unconventional superconductivity recently observed in twisted bilayer graphene (tBG) close to the magic angle. Using the Migdal-Eliashberg framework on a one-parameter effective lattice model for tBG, we show that a superconducting state can be achieved by means of collective electronic modes in tBG. We posit robust features of the theory, including an asymmetrical superconducting dome and the magnitude of the critical temperature that agree with experiments. The second half of my talk is devoted to discussing a rigorous theory for phonon-dominated transport in twisted bilayer grapheme describing its unusual signatures in the resistivity (including the variation with electron density, temperature, and twist angle) showing good quantitative agreement with recent experiments. We go well beyond the usual treatment of electron-phonon theory, including both interband and intraband processes, considering the finite-temperature dynamical screening of the electron-phonon matrix element, and going beyond the linear Dirac dispersion. Comparison of experimental data with Planckian dissipation is also shown to be inconsistent.

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IT-11

Elucidating the integrity during crisis in colloidal & emulsion droplets by SANS and SAXS

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Colloids and emulsions are ubiquitous and they form an interesting branch in science owing to the various intriguing interactions among the constituent phases. Such interactions are amalgamation of various effects, namely, electro-static, van der Waals, excluded volume, etc. As soon as the continuous medium of a colloidal dispersion *i.e.,* the solvent, starts disappearing through rapid evaporation, the interaction among the particles gets significantly altered. The extent of the modification depends on competitive dominance of the aforementioned factors. The attractive capillary force tries to setup a strong integrity among the constituent particles which are under a crisis-like situation owing to the sudden disappearance of the solvent. In fact, the process of drying of liquid droplets is widely used in various industries including food and pharmaceutical industries and this process is known as spray-drying. Since last decade, the above-mentioned industrial process has re-

embellished itself in nano-science and nano-technology. Contact-free evaporating colloidal droplets exhibit spectacular behaviors due to sudden transition from dispersion to powder state associated with assembly of the nanostructures. With the help of such evaporative assembly process, a wide variety of hierarchically structured micro/meso/macro-porous granules have been realized. Such highly correlated nanostructured micro-granules also act as hosts for investigating various nano-confinement based Physics problems owing to existence of the nanometric interstitial pores. Further, understanding of the buckling-induced shape transformation during such evaporative-assembly process remains another important aspect. Quantification of the (i) structure of these granules, extending over nanometer to micrometer length scale, and (ii) understanding of the confinement-driven time-dependent processes are crucial and challenging. Owing to their complex structure, over hierarchical length scales, it demands the use of scattering techniques accessing wide range of wave-vector transfer along with complementary imaging methods. In this regard, small-angle neutron scattering (SANS), X-ray scattering (SAXS) and scanning electron microscopy (SEM) have been found to be effective in probing such nano-structured granular materials. SANS facilities at Dhruva reactor, laboratory-based SAXS and recently commissioned SAXS beamline (BL-18) at Indus-2, RRCAT have been utilized to unravel the structural correlations in these fairly high-surface area porous granules and dendritic nanosphers. In this presentation, we will discuss some of our recent results on such hierarchically-structured granular materials and will also touch upon a few time-dependent processes in these materials.

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IT-12

A Versatile X-ray Scattering and Diffraction Beamline for Engineering Applications at Indus-2 Synchrotron Source

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A hard X-ray engineering applications beamline (BL-02) was commissioned recently and started operation in March 2019 at Indian synchrotron source, Indus-2. This bending magnet-based beamline is capable to operate in various beam modes viz; white, pink and monochromatic beam. The beamline utilizes X-ray diffraction technique in energy dispersive

and angle dispersive modes to carry out experiments mainly focused on engineering problems viz; stress measurement, texture measurement and determination of elastic constants in variety of bulk as well as thin film samples. The talk will give details of the physics design, optics, experimental stations and recent results of the beamline. Experiments executed to validate the beamline design parameters and to demonstrate the capabilities of beamline will be described. The future facilities to be incorporated to enhance the capabilities of the beamline shall be discussed.

IT-13

Creating tunable finite temperature half-metal out of an antiferromagnetic Mott insulator.

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Sustaining exotic quantum mechanical phases at high temperatures is a long-standing goal of condensed matter physics. Among them, half-metals are spin-polarized conductors that are essential for realizing room-temperature spin current sources. However, typical half-metals are low-temperature phases whose spin polarization rapidly deteriorates with temperature increase. In this talk, we will first show that a low-temperature insulator with an unequal charge gap for the two spin channels can arise from competing Mott and band insulating tendencies. We will demonstrate that thermal fluctuations can drive this insulator to a half-metal through a first-order phase transition by closing the charge gap for one spin channel. We will show within a Kubo-Greenwood transport formalism that this half-metal has 100% spin polarization at the onset temperature of metallization, and tuning the strength of electron repulsion can enhance the onset temperature while preserving spin polarization. We will end with a discussion of experimental scenarios for realizing this novel finite-temperature half-metal.

IT-14

Multiferroic properties of Pb based perovskites

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The complex Pb(B′ B″)O3 structured perovskites exhibiting multiferroic properties have gained much attention in recent years due to their potential for technological applications. For example, the Pb based complex perovskites, PbFe0.67W0.33O3 (PFW) and PbFe0.5Nb0.5O3 (PFN) shows multiferroic behaviour below certain temperatures. At room temperature, PFW and PFN exhibit cubic (Pm-3m) and monoclinic (Cm) structure, respectively. Both are antiferromagnetic with Neel temperature around 380 K for PFW and 143 K for PFN. In this talk, I will discuss the synthesis and multiferroic properties of PFN, PFW and their solid solution with another room temperature multiferroic BiFeO3 through temperature dependent Neutron diffraction, magnetization, dielectric, Mossbauer measurements. The polycrystalline PFN-PFW (PFWN), PFN- BiFeO3, PFW- BiFeO3 solid solutions were prepared through the Columbite method (solid state reaction method) with low temperature sintering technique. The nuclear and magnetic structures of solid solutions were determined by the Rietveld refinement of neutron diffraction data measured at different temperatures from 2.8 to 295 K. A possible model for antiferromagnetic order is proposed with a propagation vector k = (½, ½, ½) and the G type antiferromagnetic structure. The magnetic moment of antiferromagnetically ordered Fe3+ ions is determined and found to be μFe = 3.826 μB. The dielectric constant exhibits an anomaly around TN, which indicates

magnetoelectric coupling. These features are attributed to the inherent coupling between the ferroelectric and antiferromagnetic orders in the multiferroic system.

IT-15

Anchoring Cu(II)-Based S=1/2 Kagome Lattices on Functionalized Graphene

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Cu(II)-based atacamite family of minerals have emerged as promising candidates for the investigation of quantum spin liquid (QSL) states. Herein, starting from Cu(I) precursors, we have synthesised phase-pure Cu(II)-based S=1/2 kagome spin lattices at near-ambient conditions. When graphene oxide (GO) was taken along with other reactants, the oxidation of Cu(I) to Cu(II) was accompanied by the reduction of GO to rGO which not only led to the anchoring of various S=1/2 spin lattices onto rGO but also the magnetic exchange interactions were notably modulated by the diamagnetic rGO matrix. Overall, a series of S=1/2 kagome spin lattices are explored, all belonging to the atacamite family of minerals and are known to be antiferromagnetic insulators. Specifically, strongly coupled kagome planes (clinoatacamite), weakly coupled kagome planes (barlowite), and weakly coupled and magnetically isolated kagome planes (paratacamite and herbertsmithite) – were successfully anchored to rGO matrix. The resultant atacamite-rGO nanocomposites were assigned as magnetic semiconductors and electron doping of the kagome spin lattices by rGO is proposed.

IT-16

Phase Transitions and Disorder: A Tale of Two Scheelites

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It is the best of hettotypes. It is the worst of aristotypes. An aristotype represents the highest symmetry crystal structure that can be attained for a given system. Many inorganic systems exhibitlower symmetry phases, orhettotypes, that are crystallographically related to the aristotype as isotropy subgroups. The hettotypestructure can, therefore, be described by a symmetry-breaking distortion of the aristotype structure. The distortion contains contributions from the different modes; The correlated atomic displacements or modes that contribute to the lower symmetry are described by the irreducible representations of the aristo type space group.

High resolution powder diffraction methods, especially neutron diffraction, are well established tools for the study of phase transitions and combining such studies with group theory is a powerful approach to gain deep insight symmetry lowering in complex oxides. This talk will illustrate this using scheelite as an example. The scheelite structure is named for the Swedish chemist CarlScheele after the tetragonal structure displayed by $CaWO_4$ that is described in space group $I4_1/a$. As occurs for perovskite ($CaTiO_3$) this structure is not the aristotype, rather the WO_4 tetrahedra are rotated about the *c*-axis and the aristotype is described by space group $I4_1/amd$as seen in $RbReO_4$ at high temperatures. The irrep of the mode is Γ_3^+. Replacing the Rb with Tl in $TlReO_4$lowers the symmetry to a unique monoclinic structure and $TlReO_4$ displays phase transitions to the $I4_1/a$structure upon both heating and cooling. Such re-enterent phase transitions are unusual. PDF analysis of total neutron scattering data reveals evidence for hidden order in both the high and low temperature tetragonal forms that is associated with the stereochemical activity of the Bi $6s^2$ lone pair

electrons. The difference between the average and local structures in this and related systems will be presented.

IT-17

Jammed micelles in water-free supercooled matrix: Evidence from small angle scattering

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Amphiphilic molecules self assemble in water to form dynamic equilibrium structures such as micelles. Mostly, micelle formation is reported in liquids and undergo random Brownian motion in the solvent due to its colloidal size. However, dynamically arrested micelles can be formed by common amphiphiles in room temperature supercooled solvents. Small angle x-ray/neutron scattering provides unequivocal evidence for the formation of micelles in supercooled matrix. The micelles can be formed by dissolving an amphiphile in a molten mixture of sugar (e.g., sucrose, fructose or glucose) and urea or urea derivatives at elevated temperatures (~70-90^{o}C). These micelles get trapped in a supercooled state upon cooling the mixture to 15^{o}C, forming a sugar glass. This opens a new area of research using room temperature supercooled solvents as the matrix for micelle formation. Unlike normal micelles in water, which form only above the Kraft temperature, these micelles in sugar glass can sustain subzero degree Celsius temperatures (-25^{o}C) without phase separation. The present study shows an example of solid-like assemblies of soft materials, dispersed in another amorphous matrix. Since all components used in this formulation are solid at room temperature, the supercooled micelles can be considered as a micro-heterogeneous amorphous solid, akin to alloy formation in metals.

IT-18

Exploring the Role of Crystal Chemistry in Materials Science

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The importance of the crystal chemistry of organic solids has been well-established in the literature and the role of intermolecular interactions in this regard is of extreme relevance.1The prevalence of polymorphism is also well known in the literature2. Extensive screening for polymorphism, including solvatomorphism, in a library of small molecules containing halogen substituted ethynyl phenyl benamidesresulted in the formation of crystalline anhydrous polymorphs3, solvates of hexafluorobenzene4, and the observation of SCSC phase transitions5 in the solid state. This has relevance in associated applications as photoluminescent solids6 and dielectrics.7The current talk shall address the relevance of intermolecular interactions and the associated crystal chemistry to understand the formation of crystalline solids with diverse properties.

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IT-19

Nanostructured calcium cobalt oxide with enhanced properties for thermoelectric generation

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New materials and nanostructures are the key factors to engineer efficient devices necessary for advancement of next generation technologies. Energy harvesting and conversion of waste heat to useful form of energies could reduce the greenhouse effect resulting due to excess heat generation from various natural and artificial sources. Thermoelectric generation acknowledges a tool for converting waste heat into electrical energy by adopting sustainable, environmental friendly, and cost effective technique. Calcium cobalt oxide ($Ca_3Co_4O_9$), a misfit-layered oxide structure consisting of Ca_2CoO_3 and CoO_2 subsystems stacked alternatively along the c-axis, has been exhibiting favorable properties for considering as efficient thermoelectric material [1].

Highly pure and perfectly composed micro/nano-structures of $Ca_3Co_4O_9$ with high thermal and chemical stabilities are synthesized, consolidated them to achieve fully dense pellets using hot-press(HP) technique, and the electronic and thermoelectric behaviors are recorded using temperature dependent current-voltage, conductivity, and Seebeck coefficient measurements. Mott's 3D variable range hopping conduction at low bias region through closely packed and partially oriented textured grains formed during the HP process [2], space charge limited current at high bias region, and observation of anisotropic behaviour in the electronic resistivity are the inherent properties identified in $Ca_3Co_4O_9$ ceramics prepared using the as-synthesized microstructrues. At high temperatures of 700 K, the enhancement of around 11 times in the power factor in $Ca_3Co_4O_9$ ceramics prepared using nanostructures compared to that of as-synthesized micro-plates due to simultaneous increment of Seebeck coefficient and negligible increment in resistivity, is attributed to the raise in scattering due to introduction of more number of grain boundaries in bulk nanostructured ceramics [3]. The currently prepared nanostructured $Ca_3Co_4O_9$ demonstrates favorable properties for exhibiting enhanced thermoelectric behavior by following low cost processing techniques and could be considered for future mass-scale production for real world application.

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IT-20

Time Differential Perturbed Angular Correlation Spectroscopy: A Potential Tool to probe Materials Structure in Atomic Scale

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At Radiochemistry Laboratory (BARC), VECC, Kolkata, we have developed the Time Differential γ−γ Perturbed Angular Correlation (TDPAC) Spectroscopy consisting of CeBr3 scintillator detectors. The TDPAC is a nuclear probe technique based on hyperfine interaction where suitable radionuclide (called as "PAC Probe or Spy") is incorporated in host compound in high dilution to get the information inside the host system at the nearest neighbour of the PAC probe atom. TDPAC is an effective spectroscopic tool to determine the local structure around the probe atom and to understand the different atomic scale physico-chemical phenomena (in situ/ex situ) occurring in the host compound. Due to the sensitivity of Electric Field Gradient (EFG), TDPAC is a potential tool to identify the different intermediate phases [1] and phases with very similar lattice parameters [2] which are otherwise very difficult to be distinguished by conventional spectroscopic techniques. Different PAC probes used in the PAC studies have been produced either in Reactor at BARC or Cyclotron at VECC. The hyperfine interaction of the transition moment of nuclei with the EFG produced due to surrounding charges is utilized to obtain the atomic scale information. In the present talk, the potential application of the TDPAC in the identification of the different intermediate phases in oxide semiconductors will be discussed.

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IT-21

Microcantilevers for Ultrafast Humidity and Ultrasensitive Temperature Sensing Applications

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Microcantilevers (MC)are the simplest MEMS structures and have emerged as a promising technology for various sensing applications such as ultrasensitive mass measurements, environmental monitoring, bio-molecular sensing and detection of chemical analytes such as explosives. In this talk, our recent work on the development of ultrafast relative humidity (RH) and ultrasensitive temperature sensors using MCs will be presented. For RH sensing, micropatterned SiO_2 MCs of various dimensions were fabricated using direct laser writer and wet chemical etching methods and were tested for RH sensitivity in the range of 20% to 90% RH. It is shown that introduction of controlled micropatterns on MC surface provides aneffective way toenhance the RH sensitivity (10.45 Hz/% RH)without compromising other sensor characteristicssuch as response and recovery time(~ 1 s).These superior characteristics of micropatterned MCs allowedthe realtime monitoring of RH variation during human breathing cycles.Similarly, for temperature sensing applications, photo-induced deflection studies were carried out on Bimaterial MCs (BMC).Laser beam induced deflection in uncoated, Au, and Al coated Si MCs ofvarious dimensions was studied, using an AFM head. MC flipping experiments revealed that stress contribution in BMCscan originate either from photostriction or photothermal effects and it dependscritically on the MC dimensions and direction of laser exposure.Effect of laser parameters such as wavelength, modulating frequency and MC physical dimensions on the deflection sensitivity, response time and noise

characteristics of BMCs was carried out. It is shown that a maximum temperaturesensitivity of ~62 mK/nmand an optimum noise equivalent power of 566 pW/√Hzcan be achieved by tuning the laser parameters and BMC dimensions.

IT-22

Emergent non-Fermi liquid behaviour in disordered, strongly interacting systems

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Abstract: We provide strong evidence for a quantum critical point (QCP) associated with the destruction of Kondo screening in the Anderson-Hubbard model for interacting electrons with quenched disorder. The evidence comprises three elements: (a) the identification of an energy scale, $\omega*$, that delineates infrared Fermi-liquid damping from higher frequency non-Fermi liquid (nFL) dynamics; (b) the finding that this crossover scale $\omega*$ appears to vanish with increasing disorder; and (c) the concomitant appearance of a finite intercept in a broad distribution of Kondo scales. Our findings indicate a Kondo destruction scenario, albeit distinct from the local QCP picture. The nFL behavior is shown to stem from an interplay of strong electron-electron interactions and the systematic inclusion of short-range dynamical fluctuations induced by the underlying random potential. The results have been obtained through a computational framework based on the typical medium dynamical cluster approximation.

IT-23

Spin-orbit coupled Dirac Fermions

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One of the central quests of present condensed matter research is to find new phases of quantum matter. In this regard, a crucial ingredient is the emergence of novel implementation of symmetries. In this talk, I shall discuss how new and enhanced symmetries may arise at low energies in a two dimensional honeycomb system due to spin-orbit coupling in certain heavier transition metal compounds. The resultant Dirac semimetal phases, as I shall discuss, act as parent phases for several unconventional topological phases and associated phase transitions.

IT-24

Strong Electronic Correlations Observed in Colossal Thermoelectric Material K0.65RhO2 Using Angle-Resolved Photoelectron Spectroscopy (ARPES)

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Using angle-resolved photoemission spectroscopy (ARPES) and density functional theory (DFT) calculations we studied the low-energy electronic band structure of K0.65RhO2. We identify a highly correlated hole pocket on the Fermi surface of K0.65RhO2. Most importantly, two kinks at the binding energies of 75 and 195 meV have been observed below the Fermi level. While the low-energy kink at 75 meV can be understood as a result of the electron-phonon interaction, the high-energy kink at 195 meV is a new finding of this system, leading to anomalous band renormalization, possibly originated from the bosonic excitations

at higher frequencies. We further notice that the high-energy anomaly has important implications on the colossal thermoelectric power of K0.65RhO2.

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IT-25

Spin-orbitronics: Interconversion between charge and spin currents

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Interconversion between charge and spin currents has attracted great research interest in the past decade1,2. Spin-orbit interaction at the interface between ferromagnet/non-magnetic materials is at the basis of the recent advances in pure spin current based spintronics devices such as spin-orbit torque magnetic random access memory (SOT-MRAM). In-plane current through a non-magnetic materials can generate transverse spin current via spin Hall effect that leads the switching of adjacent ferromagnetic layer. The efficiency of charge to spin conversion strongly depends on the spin-orbit coupling (SOC) of the non-magnetic layers which can be quantified from spin Hall angle, ratio of spin current to charge current. In this talk, I will demonstrate the spin-orbit torque induced switching in (Co/Ni) ferromagnetic layers adjacent to a heavy metal Ta. The effect of Ta layer thickness on the efficiency of the switching will be presented. Later, I will discuss about the possibility of using rare-earth metals to harvest spin currents due to relatively large SOC. The SOT switching between (Co/Ni)/Ta and (Co/Ni)/Tb are systematically compared in our study3. The spin Hall angle of Tb is found to be 3 times higher as compared to the conventional heavy metals. I will discuss about the spin-orbit torque based reconfigurable logic we have proposed and demonstrated4. The second part of my talk I will discuss about our recent studies on the spin to charge conversion via spin-pumping experiments in ferromagnetic/heavy metal interfaces. The detailed study of systematic investigation of the effect of seed layer on the crystalline phase and spin Hall angle of the heavy metal will be presented5.

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IT-26

Defect induced Non-ergodic Ground States in Martensites

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Point defects above a critical concentration suppress the long-range order and realise in a non-ergodic state like glass. This is true for a crystal to glass, ferromagnet to spin glass, ferroelectric to a relaxer or martensite to strain glass. Though there are several studies on

glass transition, very few studies focus on identifying the defect phase and understanding the structural distortions caused by the doped impurities. Using Extended X-ray Absorption Fine Structure (EXAFS) and other structural probes we elucidate the structure of the defect phases and the structural distortions responsible for strain glassstate in the martensitic alloys.

In Ni-rich NiTi, the body-centred cubic Ni defect phase embedded among the B19' martensitic NiTi grains is responsible for martensite to strain glass transition [1]. A similar defect phase, cubic □-FeNi, results ina strain glass state in $Ni_2Mn_{1.5-x}Fe_xIn_{0.5}$[2]. We also discuss scenarios of martensite to ferromagnetic austenite transformationin doped Heusler martensites [2,3].

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IT-27

Tailoring the properties of composites with carbon nanomaterials as reinforcement

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Carbon nanomaterials can have wide range of structures and properties namely, 'zero' dimensional carbon dot, 'one' dimensional carbon nanotube, 'two' dimensional graphene and 'three' dimensional nanodiamond. These nanomaterials when incorporated into polymer matrix, metal matrix and ceramic matrix composites, alter the properties in these composites. The microstructure and the properties can be tailored by controlling the composition and the processing parameters. This talk will showcase several such applications carried out in our group, where tremendous improvement in specific properties could be achieved through reinforcement with carbon nanomaterials.

IT-28

Positron beam studies on the Irradiation damage resistance in High entropy alloys

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High entropy alloys (HEAs) are a family of multi elemental alloy systems containing more than four elements in near/equiatomic proportions [1]. In HEA, all the elements are principal elements and the high configurational entropy which arises due to the presence of multiple elements, drives the alloy system to form a random solid solution having a simple FCC, BCC, or HCP structure rather than forming intermetallics [1]. The application of HEA as a nuclear structural material has driven a lot of research works into understanding the defect microstructures produced upon heavy ion implantation using Transmission electron microscopy technique, as the major workhorse [2]. Similarly, molecular dynamic simulation studies have also been carried out to support the experimental findings and provide insights into the defect evolution and the microstructural response of the system with elevated temperatures [3]. All these experimental findings show high phase stability, improved resistance to radiation-induced segregation, void swelling, and helium bubble growth [4].

Positron annihilation spectroscopy (PAS) is an excellent non destructive defect characterization tool which can detect vacancy defects starting from monovacancy to small vacancy clusters to voids [5]. Variable low energy positron beam setup at IGCAR, Kalpakkam enables non- destructive depth profiling of implantation induced defects such as

vacancy defects, stacking fault tetrahedrons (SFT), voids, helium bubbles etc., up to a depth of few hundreds of nm of the material [6].

This talk will focus on the application of the HEA as a reactor structural material citing the recent research works and also quoting some of our experimental findings relating to the implantation induced defects in FeCrCoNi using the variable low energy positron beam setup [7].

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IT-29

Doping site induced modification of the magnetic structure of MnNiGe alloys

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The magnetic equiatomic alloys (MEAs) with general formula MM′X (M/M′ = transition metals, and X = non-magnetic sp element) and their derivatives haverecently been identified as the new shape memory alloy class. Apart from the shape memory effect, various interesting magneto-functional properties are also associated with MEAs, including giant magnetocaloric effect, large magnetoresistance, exchange bias effect, magnetic memory, etc. Among MEAs, MnNiGe is the most studied one. The pristine MnNiGe alloy undergoesa martensitic phase transition (MPT) around 470 K and orders antiferromagnetically below 346 K. For enhanced magneto-functionality, the researchers have adopted several doping strategies. Some of such strategies are (i) doping of foreign elements in Mn/Ni/Ge sites, (ii) self doping, (iii) creation of vacancy in Mn/Ni/Ge sites, (iv) application of external pressure (P), etc. The main aim behind such strategies is to reduce the martensitic phase transition below or around the magnetic transition temperature for enhanced magneto-functionality. In the case of foreign element doping, dc magnetic investigation indicates that the magnetic nature of different phases depends strongly on the doping sites. For Ni/Mn site doping cases, the doped alloys undergo magnetic and structural transitions simultaneously. On the other hand, Ge-site doped alloys undergo a martensitic transition in the magnetically ordered austenite phase. Previous neutron powder diffraction (NPD) studies indicate the spiral antiferromagnetic structure of pure MnNiGe alloy. However, very few NPD studies have been performed to explore the magnetic structure of doped MnNiGe alloys. This work aims to probe the effect of foreign element doping at Mn, Ni, and Ge siteson the magnetic structure through NPD study in ambient and high-pressure conditions. In the case of Ge-site doping, we observed a commensurate to incommensurate antiferromagnetic transition around MPT. Interestingly, both Ni and Ge site doped alloys show helically modulated incommensurate antiferromagnetic structure, whilst, a cycloidal modulation has been observed for the incommensurate antiferromagnetic structure of the Mn site doped alloy. A significant change in magnetic structure has also been noticedin the presence of external pressure.

IT-30

Pressure tuning of material properties: selected examples from the joint Indo-Italian beamline "Xpress" at Elettra–Synchrotron Trieste.

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Pressure is a thermodynamic variable extremely useful in altering the material properties. For condensed matter physicist tuning of the electronic properties are of utmost important; for chemist, it is the bonding properties and for the material scientist, the functional properties. In all such cases, high-pressure from few to few tens of giga-Pascal (GPa) are found to be of great use. We elaborate this by discussing three different systems: First, we discuss the pressure effects on the suppression of a charge density wave transition in LaAuSb2 and its connection to the structural degrees of freedom [1]. We then present inputs from the high-pressure diffraction on the occurrence of meta-valent bonding state in doped GeSe [2]. In the third example, we demonstrate the realization of a novel hybrid nanocomposite with interesting gas sensing properties using combined pressure-temperature treatment of a porous system [3]. Excellent high-pressure diffraction data were essential in all the above cited examples which were available thanks to the Indo-Italian high-pressure diffraction beamline facility – Xpress, at the Elettra synchrotron radiation center at Trieste. The salient features of this facility will be presented. In particular, citing few recent scientific out-puts from the Indian research groups [1,2,4,5], the broader appeal of the facility, also to non-specialists of the high-pressure field, will be high-lighted.

This presentation will also provide a brief introduction to the Elettra synchrotron radiation facility, the Indo-Italian collaboration existing there and the opportunities for the Indian user community in availing this facility.

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IT-31

Thermodynamic Behaviour of Graphite Under Extreme Conditions of Nuclear Radiation, Pressure and Temperature

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Graphite is used as a moderator and reflector material in nuclear fission reactors. Graphite also serves as a non-replaceable structural component in reactor cores, which must remain stable over the lifetime of the reactor while operating at elevated temperatures. In a reactor, neutron irradiation damage in graphite results in the formation of structural defects, such as displaced atoms, vacancies, and higher order aggregates that raise the internal energy. Relaxation of the defects leads to spontaneous release of energy at around 473 K, which is referred as Wigner energy. This stored energy associated with defects can surprisingly reach large energy densities with values as high as 2.7 MJ/kg. The bursts of released energies may be intense enough to cause fires in reactor and lead to nuclear accident. Recently we have thoroughly investigated thermodynamic behaviour of graphite under extreme conditions of

nuclear radiation, pressure and temperature by numerous experiments and ab-initio simulations.

We have investigated graphite samples that had been irradiated with neutrons at various levels of fluence in the CIRUS research reactor at Trombay, India over a period of almost 50 years. We have performed neutron diffraction, X-ray diffraction, small-angle X-ray scattering, Raman scattering, differential scanning calorimetry and specific heat measurements, which have been complemented by state-of-the-art ab-initio simulations of the defect structure and dynamics. We have identified various 2-, 3- and 4-coodinated topological structures at atomic level in defected graphite, and provided microscopic mechanism of defect annihilation on heating and release of the Wigner energy. Our studies showed that the annihilation process involves cascading cooperative movement of atoms in multiple steps involving an intermediate structure [1]. Neutron diffraction studies revealed [2] persistence of some of the defects in graphite at high temperatures much greater than 653 K, where the Wigner energy is completely released. We infer that the remnant defects may be intralayer Frenkel defects, which do not store large energy, unlike the interlayer Frenkel defects that store the Wigner energy. The experimental observations are complemented by ab-initio calculations [2].

We have also investigated the anisotropic thermal expansion of graphite using ab-initio calculations [3] of phonons. We find that the negative thermal expansion (NTE) in the a-b plane below 600 K and very large positive thermal expansion along the c-axis up to high temperatures arise due to various phonons polarized along the c-axis. While the NTE arises from the anharmonicity of transverse phonons over a broad energy range up to 60 meV, the large positive expansion along the c-axis occurs largely due to the longitudinal optic phonon modes around 16 meV.

Static compression of hexagonal graphite (HG) results in transformation to hexagonal diamond (HD) or cubic diamond (CD) over wide range of pressure and temperature. Recent shock studies of the transition from HG to HD or CD have created much interest in understanding the mechanism of these transitions. The nucleation and growth mechanism of these phase transitions, as found in static experiments, has been investigated in literature. However, the transition in shock experiments occurs at a fast time scale of ~ps, and may involve a different mechanism. We have used ab-initio molecular dynamics simulations [4] to elucidate the mechanism of the phase transition in shock experiments from hexagonal graphite (HG) to hexagonal diamond (HD) or to cubic diamond (CD). The transition from HG to HD is found to occur swiftly in very small time of 0.2 ps, with large cooperative displacements of all the atoms. We have also performed calculations of the phonon spectrum in HG at high pressure, which reveal soft phonon modes that may facilitate the phase transition involving the sliding and puckering of the HG layers. We have further calculated the Gibbs free energy, including the vibrational energy and entropy, and derived the phase diagram between HG and CD phases.

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IT-32

Recent advances in the study of plastic strain induced phase transitions under high pressures

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In conventional hydrostatic or quasi-hydrostatic high-pressure studies, phase transitions (PT) are mostly pressure or stress induced. These PTs initiate at pre-existing defects or nucleation sites below the yield. Whereas, under high-pressure torsion (HPT) new defects are permanently generated during plastic flow. This leads to much more dislocations in a pileup and may drastically reduce PT pressure, sometimes even by two orders of magnitude. These plastic strain induced PTs require completely different thermodynamic treatment and experimental characterization [1-3]. Rotational diamond anvil cell (RDAC) [4] which are similar to conventional diamond anvil cell (DAC), but with additional degree of freedom of rotation of one anvil with respect to another, are best suited for these studies. I will present some of the recent developments for quantitative experimental characterization of plastic strain induced phase transition along with a few representative studies on metallic [5] and non-metallic systems.

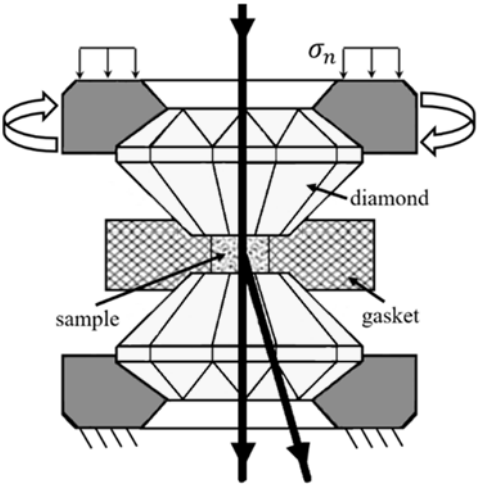

Fig. Schematics of rotational diamond anvil cell.

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IT-33

Experimental evidence of a novel anomalous transport regime in hybrid, non-Hermitian disordered systems.

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Non-Hermiticity modifies the transport properties of complex systems in various intriguing ways. In this work, we report an anomalous transport regime wherein an unexpected rise in transmission of hybrid quasiparticles is observed under localizing disorder. The behavior can be traced to the confluence of hybridization and non-Hermiticity, in which the former results into the formation of a miniband of eigenvalues under disorder, while the latter allows hopping of the quasiparticles between the eigenmodes. The enhanced transmission is facilitated by the formation of necklace states in the Anderson localizing system. We demonstrate experimental results confirming the anomalous regime at microwave frequencies in a one-dimensional spoof surface plasmonic system.

IT-34

Graphene drum resonators coupled over long distances: towards controlled phononic time crystals

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Suspended graphene membranes provided a powerful NEMS platform for envisioning new technologies and in exploring science at the interface of strong mechanical nonlinearity and quantum dynamics. Here we will argue with three examples from our laboratory on the versatility of graphene resonators for such platforms. Firstly, we will demonstrate graphene as a motion sensor that can be used to detect femto-meters of displacement induced on a Silicon Nitride(SiN) substrate, which is also a resonator (1). In the second example, we will discuss how one can induce a large nonlinear response on SiN resonator mode, along with a novel frequency comb signature, by coupling it to graphene modes (2). Finally, we will discuss a novel mechanism of coupling two distant graphene resonators, separated by 40 microns, via the intermediate SiN resonator modes. We found a new dynamical phase, where persistent beats or frequency combs in the spectra coexist with synchronization of the two distant drum resonators (3). Such coupling between two drums can be readily extended, towards realizing large area phononic time crystals, with controllable dispersion and response.

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IT-35

Organic Photodetector As Next Generation Light Detection: Challenges And Opportunities

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One of the important optoelectronic components is photodetector whose performance significantly influences the performance of the whole optoelectronic integrated components. The photodetector provides a great solution to global challenges in energy, health care, communication, information processing., remote control, industrial automation, night surveillance, environmental monitoring, biological detection and so forth [1-3]. A high-performance photo-detector should satisfy the **5S** requirements of **S**ensitivity, **S**ignal-to-noise ratio, spectral **S**electivity, **S**peed, and **S**tability. Those **5S** requirements have been reasonably optimized in traditional inorganic photodetectors and has led them to form the base of present-day light-detection technology. However, their *rigid structure* and *limited area scaling at low cost* have hindered their application in several emerging fields, such as context-aware optical sensing, touch less interactive computing, wearable biometric monitoring, biomedical imaging, distributed ionizing-radiation detection etc. Furthermore, *complicated manufacturing process* and *less effectiveness in cost-saving* have also restricted their applications. In this direction, *'Sensors'* based on organic photodiodes have become one of the most innovative technologies [2-7].

There are several advantages of organic photodetector (OPD) over inorganic photodetector:

- Light weight, mechanical flexibility and compatibility with large and rigid substrate.
- Ease of production, chemical modification and easy to fabricate at low temperature.
- Large *optical absorption coefficients* (10^5/cm).
- *Organic optoelectronic devices are more Energy Efficient and Eco friendly.*

Such devices can be easily integrated into various systems, such as flexible, wearable or portable electronics. Recent research has demonstrated reasonably well figures of merit of organic photodetectors, compared to common inorganic photodetectors in the area of ♦ wider dynamic range; ♦ broader spectral range; ♦ better responsivity.

Organic Photodectors also bear a potential market worldwide. According to the report of *Research Reports World*, Organic Photodetectors can have widespread implications for many markets for consumers and enterprises [8]. Manufacturers across industries are constantly researching for ways to develop newer functionalities in their products. Moreover, a change in the base material itself would be at the base of a range of further innovations. An attitude of developing ground breaking innovations is therefore fueling the research happening towards Organic Photodetectors. The major players in Organic Photodetector market include ISORG, Silvaco, Inc, NikkoIA SAS, OSRAM GmbH, & Albis Optoelectronics AG.

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IT-36

Defect mediated multicolored emission from pristine ZnO nanostructure: A voyage towards single source white LED

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Recently, UV/NUV excitable RGB phosphors with precisely tuneable PL emission properties have been in highdemand for their suitability in the fabrication of white LEDs. We have tried with success to generate for the first-time multiple emission havingtuneable PL intensity, shade, and color temperature in pristine zinc oxide. The ZnO nanopowder was prepared by a facile and cost-effective aqueous solution-precipitation method. The as-synthesized nanopowder was annealed at different temperatures ranging from 150 _C to 850 _C and all these samples were characterized by XRD, FESEM, EDX, BET, Raman spectroscopy, and UV-Vis spectroscopy to have insight into their microstructural, compositional, and band-structure details. Optical studies of the samples were conducted using PL and s-PL spectroscopy. Color coordinates of the samples were obtained from the CIE plots derived from the PL spectra. The CIE coordinates were further used to calculate the CCT values of the samples and they are found to be suitable in cold light applications.These nanostructured zinc oxide particles being sufficiently large in size are extremely stable and expected to show photoluminescence for a longer period of time than nanorods and quantum dots. PL studies of the samples revealed that various emission is originating from crystalline point defects, viz. zinc interstitial (Zni), and oxygen interstitial (Oi). Annealing at different temperatures triggered changes in the defect concentrations leading to the corresponding changes in the intensity, shade, and color temperature of the blue phosphorescence.

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IT-37

Surface Micro Engineering of Silicon for Efficient and Cost Effective PEDOT:PSS/Silicon Hybrid Solar Cells

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Solar photovoltaic (SPV), which is dominated by silicon (Si) based homojunction solar cells, is one of the most reliable technologies for harvesting solar energy. However, these PV cells are based on high thermal budget dopant-diffusion and annealing processes (≥850°C), in

atmosphere of phosphorus or boron, depending upon type of impurity in Si wafer) [1, 2, 3]. Naturally, these processes are time consuming, complex and in turn increase per unit power cost of the SPV devices. This has driven significant research interests towards combining the best of both organic and inorganic systems. Organic carrier selective layer with Si is a promising approach for the next generation of cost-effective solar cells owing to their unique properties like light weight, cost effectiveness and environment friendly [4, 5]. The organic/Si hybrid solar cells (HSCs), in principle, can achieve comparable efficiency to that of a conventional Si homojunction solar cell as light absorption and photo-carriers generation take place in the Si wafer only in such HSCs architecture [4].

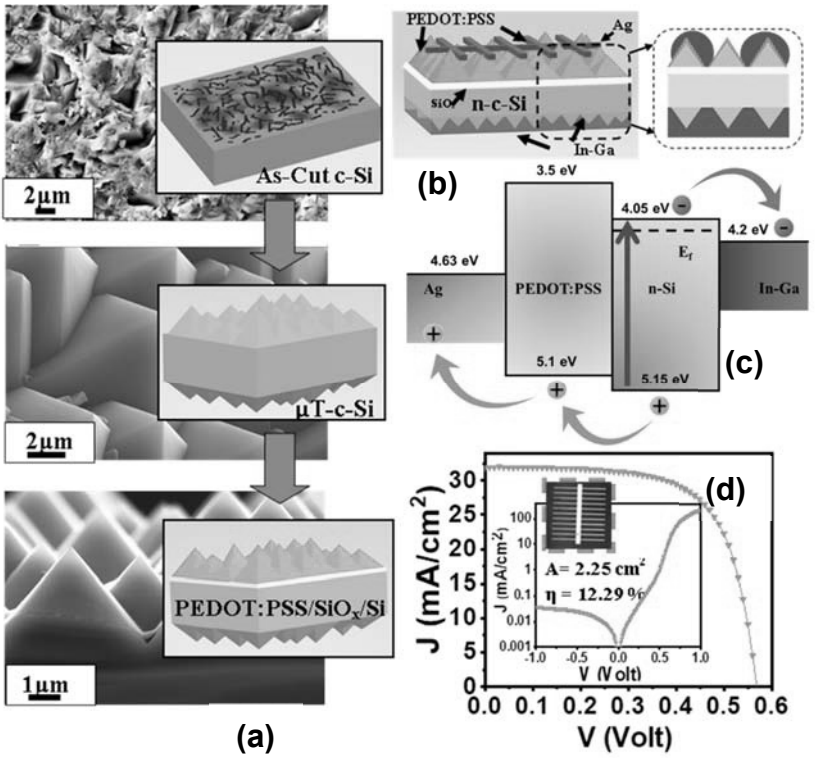

Figure 1:(a) Schematic of process flow of making of micro-structured Si surface from the as-cut solar grade Si wafers and PEDOT:PSS/n-Si interface(junction), (b) Schematic of hybrid solar cell device structure (Ag/PEDOT:PSS/-n-Si/In:Ga), (c) schematic of the operation principle of such HSCs, and (d) solar cell performance characteristics of the champion HSC.

Most commonly, an inexpensive, highly conducting and transparent polymer namely, poly(3,4-ethylenedioxythiophene)-poly(styrene sulfonate) (PEDOT:PSS), which acts as a p-layer (carrier selective hole transport) is coated over n-type crystalline Si surfaces resulting into a Schottky junction at the PEDOT:PSS/Si interface [4, 5].The PEDOT:PSS is suggested to play four vital roles in such HSCs, namely; (i) it induces an inversion layer in n-Si (i.e., a p-dopant-free, Si p–n junction is formed) to block electrons and extract holes, (ii) it transports holes to the metal anode, (iii) it acts as a surface passivation layer to reduce interfacial recombination, and (iv) it increases light harvesting by reducing reflection losses. The HSCs

based on PEDOT:PSS/n-Si, have attracted a lot of attention toward the development of low-cost and efficient photovoltaic devices.

However, it requires extensive control and optimization of the photoelectric property of the PEDOT:PSS thin films, Si surface properties,PEDOT:PSS/n-Si hetero-interface, n-Si/rear electrode contact, and so on. An appropriate PEDOT:PSS/Si interface formation and its properties are key to achieve high-performance solar cells. Effective surface nano/micro-engineering of the Si wafers, can play important role in achieving not only effective light harvesting but also a quality PEDOT:PSS/n-Si hetero-interface leading to high efficiency HSCs [6]. For example, recently highly efficient PEDOT:PSS/Si HSCs (with photo-conversion efficiency >12.25%) could be achieved via an effective surface micro-engineering of the as-cut, low-cost solar-grade thin Si wafers, by a simple one-step aqueous KOH process (see Fig. 1). The process reduces the weighted surface reflectivity from >35% to <9% in broad spectral range in addition to removing the surface saw-damages of the wafers completely. The combined effect in turn improves the PEDOT:PSS/Si interface (junction) property leading to a highly efficient PEDOT:PSS/Si HSCs even in its simplest possible device structure.

Thus, a simple yet efficient HSCs on such economic solar-grade Si wafers, commonly used for the conventional Si solar cells, could be demonstrated. Further, it is shown that effective micro-engineering of the commercial as-cut Si wafers removes the surface-damages on both sides which if not addressedproperly, cause very high surface recombination losses and has detrimental effect on the polymer/Si junction and hence the PV performances. The talk will discussfew such examples of efficient hybrid solar cellarchitectures employing different simple and cost effective micro-and nano-structuring schemes of Si wafers, carried out at CSIR-NPL during past 5 years.

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IT-38

Probing Magnetic Properties of Oxides Thin Films Using XMCD Studies at Indus-2 Synchrotron Source

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The wide range of exotic structural, electronic, dielectric and magnetic properties exhibited by the transition metal oxides (TMOs) emanate from the competing forces encountered by transition metal (TM)-3*d* electrons, such as electron-electron Coulombic interaction which favors localization of electrons, and TM 3*d*-O 2*p* hybridization which facilitates the electrons delocalization. Strain engineering in thin films of these materials provides a window to tune

these parameters and hence control over their electronic and magnetic ground states. It is of huge importance and fundamental in nature to ascertain an unequivocal origin of modifications in the electrical, electronic and magnetic properties of these films or their hetero-structures, in order to tune their properties. A comprehensive study using resonant photoemission spectroscopy (RPES), X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD) experiments, which are feasible at Indus synchrotron sources at RRCAT, Indore, allows us to unravel the coupling among structural, electronic and magnetic properties. We take an example of orthorhombic brownmillerite (BM) $SrCoO_{2.5}$ (SCO), which is an antiferromagnetic insulator in bulk form. The RPES studies reveal that the electronic ground state of the system transforms from $3d^n$ in bulk to $3d^{n+1}\underline{L}$ ($\underline{L}$: O-2p hole) in the strained thin film due to enhanced hybridization strength. XAS and XMCD experiments performed at Indus-2 synchrotron source reveal that the strained SCO thin films possess negative charge transfer energy (Δ) value and it transforms from antiferromagnetic in bulk to ferromagnetic in the strained thin film. The induced ferromagnetism is described in terms of the negative Δ, O-2p hole density, and charge & spin-state disproportionation in the system. Interestingly, when this ferromagnetic strained SCO film is integrated with another ferromagnetic $La_{0.7}Sr_{0.3}MnO_3$ film, the heterostructure reveals unusual exchange biasing. The electronic, orbital, and spin reconstruction taking place at the interface between these two ferromagnetic oxides materials lead to an antiferromagnetic interaction between the moments at Mn site and Co site across the interface, as divulged from the XMCD studies.

IT-39

Unique Magnetotransport in KTaO3 based conducting interfaces: Planar Hall effect, Anomalus Hall effect, Shubnikov-de Haas oscillations, Berry's phase, Chiral Anomaly(?)

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Abstract: In recent times, momentum dependent splitting of spin-bands in an electronic system, the "Rashba effect", has gained a lot of interest because of its applications in future generation spintronic devices.[1,2] The Rashba effect is important not only because it has tremendous potential for technical applications, but also it is a hunting ground of emergent physical properties owing to the linear dispersion relation at the crossing point of the two spin bands.[3] In this work, we present observation of emergent phenomena arising at the interface of two insulating perovskite oxides due to Rashba spinband splitting. In our first work, we improvise a novel conducting interface by juxtaposing KTaO3 (KTO) with another insulator, namely LaVO3 (LVO).[4] This heterointerface exhibits strong spin-orbit coupling which is the highest among perovskite oxide heterostructures reported so far. The system is also found to show signature of topological chiral anomaly via observation planar Hall effect (PHE) and anomalous inplane magnetoresistance (AMR) similar to that observed for topological systems. [5] In our next work, we show the realization of conducting interface between ferromagnetic EuO and non-magnetic KTO. [6] This heterostructure is found to exhibit Shubnikov-de Haas oscillations. The observed oscillations suggest the presence of two Fermi surfaces. For both the Fermi surfaces, we have seen the presence of a non-trivial "Berry phase" suggesting that the surfaces enclose a "Dirac point" and the Berry phase originates from the inner and outer Fermi surfaces of the Rashba spin-split bands. Analysing the SdH, Hall and magnetoresistance data, we have drawn a possible band diagram near the Fermi surface for EuO-KTO heterointerface. Our observations suggest that perovskite oxides with strong spin orbit coupling and relativistic conduction electrons could be a hunting ground not only for spintronic materials but also for emergent physics.

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IT-40

Engineering van der Waals solids for tunable optical and electronic properties

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Atomically thin two dimensional (2D) van der Waals (vdW) solids, especially transition metal dichalcogenides (TMDCs) have attracted prodigious attention to the versatile research in semiconductor technologies, nearly outclassing conventional semiconductors owing to their excellent physical properties. The layer dependent variable bandgap, strong spin orbit coupling, interlayer twist-angle in vdW heterostructures provide multiple degrees of freedom to probe various electronic, optical and thermal properties. In this talk, I will discuss about growth of large scale, high quality monolayer MoS_2 towards the realization of high-performance hysteresis free field-effect transistor. Minimization of the charge trapping under pulsed I~V measurements, provides the intrinsic transistor behavior with record high mobility.[1] Moreover, the generated moiré patterns in twisted bilayer MoS_2 modify the lattice dynamics through periodic potential, which enable pathways to control the phonon-phonon interactions and quantum behaviors in vdW heterostructures. Electric field modulated carrier transfer in MoX_2/WX_2 heterostructures with varying stacking geometries can be achieved for efficient performances in optoelectronic devices.[2]

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IT-41

Lithium based Battery: Fundamentals and Challenges Ahead

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Lithium-ion battery is the latest addition to the family of rechargeable battery type. These batteries use intercalated lithium compounds as the electrode materials. Different cathode materials like $LiCoO_2$, $LiMn_2O_4$, $LiCo_{1/3}Mn_{1/3}Ni_{1/3}O_2$, $LiFePO_4$ have been tried in recent past. Among these cathodes, $LiFePO_4$ has become most attractive cathode material due to safety, low cost, low toxicity, stable voltage platform and long cycle life. However, due to poor electronic conductivity and slow diffusion of lithium ion in pure $LiFePO_4$, restrict its use for wide applications. The use of nanosize $LiFePO_4$ allows for fast lithium diffusion and to improve the electronic conductivity, few important approaches have been proposed like coating the particles with a conductive film of carbon or wrapping the particles with graphene, and doping with aliovalent or isovalent ions. In the anode side, molybdenum-based electrodes like MoS_2 and Mo_2C are found to be suitable candidates for lithium ion battery. The intercalation and deintercalation mechanism have also been derived using different techniques. The futuristic lithium-based battery will be of Li-S battery due to higher energy density. In those batteries the issues are low cycle life due to dissolution of sulphur in the electrolyte. However, by suitable modification in the electrode and electrolyte the dissolution can be minimized.

IT-42

Surface modification by metal-oxide nanoparticle coatings for improving the cycling characteristics of the cathode material

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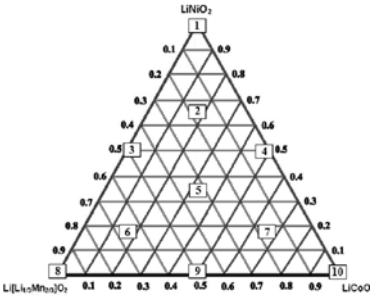
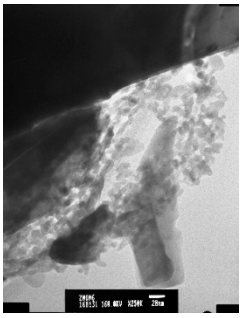
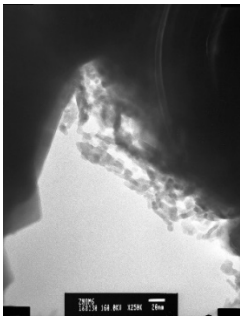
The cathode materials in the ternary system (1-x-y) $LiNiO_2 \cdot xLi_2MnO_3 \cdot yLiCoO_2$ shown in the diagram are obtained through scalable, co-precipitation followed by solid state reaction at 975 °C. The compositions on the ternary diagram {a combination of $LiNiO_2$, Li_2MnO_3, and $LiCoO_2$ layered structures} are chosen through an arrangement conducive to mathematical modelling. The X-ray diffraction studies on the synthesised materials confirm the α-$NaFeO_2$ structure, except in compositions close to $LiNiO_2$ on the ternary. Through electrochemical testing revealed the specific capacity from 150 to 250 mAh/g for different samples based on their compositions. The samples with high manganese concentration delivered higher capacity in excess of 225 mAh/g in the first cycle, however, the subsequent cycles resulted capacity fading. We have tried to modify the surface of these cathode materials in order to increase the capacity retention. Metal oxide (Al_2O_3, ZnO, $AlPO_4$) nanoparticles are separately coated and the capacity retention is compared. Differential scanning calorimetry (DSC) testing on this material was promising as it showed an exothermic reaction of 0.2 W/g at 200° C when tested up to 400° C. Cost for laboratory quantities of material yielded $1.49/Ah, which is significantly lower than the cost of $LiCoO_2$ due to the low cobalt content, and the straightforward synthesis.







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IT-43

Designing of Carbon Based Energy Material

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This talk aims to explore the promising applications of several carbon allotropies and its structural derivatives in the field of energy[1,2]. The intrinsic band gap of these allotropies are occasionally tuned to suits for technological applications. Using density functional theory methodology, structural and electronic properties of these materials will be discussed with special emphasis on nanoscale capacitor and anode-material designing. How doping affects these properties will also be analysed. A novel two-dimensional carbon material, namely pentagraphyne[1] is proposed which is energetically favourable than other graphyne members. Remarkable carrier mobility along with its superior optical performance renders it to be a potential candidate for future electronics, photovoltaic solar cells, and optoelectronic devices. Graphyne, twin-graphene and pentagraphyne immerged as an excellent candidates for nanocapacitor[3-5] Na-ion battery[6,7] and thermoelectricity[8].

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CONTRIBUTORY PAPERS

a: PHASE TRANSITIONS AND DYNAMICS

a0001

Dielectric Relaxation Investigations In A Ferroelectric Liquid Crystal

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Dielectric relaxations in a ferroelectric liquid crystal namely Camphoric acid (CA) reacted with alkyloxy benzoic acid (BAO) and the resultant homologous series of HBFLC is discussed. The mesogen exhibits smectic C* and smectic G* phases. Arrhenius plots are constructed in smectic C* phase elucidating data from eighteen temperatures which covers the entire thermal span of smectic C*. A molecular modelling of the mesogen is given which gives the explanation for various relaxation frequencies.

a0002

Effect of Electron-Hole Concentration On The Self-Trapping Transition Of Polaron In the Presence Of Strong Coulomb Correlation

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The two-dimensional Holstein-Hubbard model has been studied for the strongly correlated electrons. A series of canonical transformations have been performed followed by an averaging with the generalized all phonon state to eliminate the phonon degrees of freedom. In order to study the system in the strongly correlated regime, the electronic Hamiltonian is transformed to an effective t-J model and using the Hartree-Fock approximation, the ground state energy of the system is solved with numerical variational technique by the use of Zuberev's Green's function method. It has been found that the polaronic mobility ceases as the electronic concentration in the system increases and with the strengthening of the on-site electron-phonon interaction, the polaron gets trapped in its own potential at lower electronic density. The study of the on-site variational parameter with respect to the on-site electron-phonon correlation strength implied strong electron-phonon interaction is required for the higher hole concentration.

a0003

Omnipresent instability criterion of birefringent Kundu-Eckhaus model with nonic nonlinearity

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We investigate the modulational instability (MI) in a coupled birefringent Kundu-Eckhaus (KE) model with the help of pulse propagation technique. Using standard linear stability method, we detail study the effect of both self and cross phase modulation of KE fiber system without four wave mixing term. Also, we investigate the impact of nonic nonlinearity in a coupled birefringent media with the support of contour image through dispersion relation for small perturbation. Using omnipresent modulational instability criteria, the coss phase modulation and self phase modulation effects on optical wave propagation in birefringent fiber are discussed in the presence of both cubic and nonic nonlinear term.

a0005

Amorphous-Crystalline Phase Induced Properties Change Of $In_{15}Sb_{10}S_{15}Se_{60}$ Thin Films Upon Thermal Annealing

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The present study reports the amorphous to crystalline phase transformation by thermal annealing at different temperatures and related optical properties change in $In_{15}Sb_{10}S_{15}Se_{60}$ thin films. The different phases developed with annealing temperature as found from the XRD and the related surface morphology were noticed from the FESEM data. The bandgap reduced and the refractive index increased with annealing. The influence of temperature on the variation of different parameters were elaborately explained on the basis of defect states in localized region. The optical conductivity and electrical conductivity both increased with annealing.

a0006
Topological Phase Transition at Quantum Criticality
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The physics of edge modes is an intriguing phenomenon observed in topological materials such as topological insulators and superconductors. Finite bulk gap facilitates the existence of theses edge states. Recently, the topological states of matter have witnessed a new physical phenomenon where gapless edge and bulk excitations coexist. This implies the presence of exponentially localized edge modes even at criticalities. The criticalities with topological and non-topological properties enable one to look into an unprecedented and interesting multicritical phenomenon: topological phase transition at criticality. We explore the existence of such topological transition and develop a suitable theoretical framework to characterize them based on the diverging nature of the curvature function.

a0009
Quantitative Phase Fraction Analysis of Ball Milled FeSiB Powder Mixture using the Rietveld Method: Effect of Micro-absorption
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X-ray diffraction (XRD) based Rietveld method is commonly used for quantitative determination of crystalline phase fractions in a powder mixture containing multi-phase components. The accuracy and reliability of this method is strongly dependent on the relative (X-ray) micro-absorption effects of particles of various phases present in the mixture. In multi-phase Rietveld refinement proper correction is required to account for this effect. This effect is known by the Brindley particle absorption contrast effect in literature. In this work a mixture of elemental Fe, Si and B powder is studied using Cu K_α radiation source and effect of micro-absorption on quantitative phase fraction analysis is discussed.

a0010
Investigation of Piezoelectricity and Photoluminescence in Eu Doped $(N_{0.41}K_{0.09}Bi_{0.5})TiO_3$

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The piezoelectric and photoluminescence response has been investigated for europium doped NKBT ($Na_{0.41}K_{0.09}Bi_{0.5}TiO_3$) ceramics. The optimum piezoelectric response was observed for 1.0 at.% europium doping, afterwards a gradual fall in the piezoelectric response was evident. On the contrary photoluminescence intensity increases with the increase in the europium content. No quenching effect was observed in the luminescence intensity till 3.0 at.%. The results are explained on the basis of amphoteric nature of europium and lack of direct correlation between photo-luminescence and piezoelectricity.

a0011
Effect of temperature on the phase formation of pure ($BaFe_{12}O_{19}$) and zinc-zirconium co-doped barium hexaferrite ($BaZnZrFe_{10}O_{19}$) samples using Rietveld analysis.
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From a performance standpoint, structural changes in ferrites that occur as a result of doping and increased processing temperature are critical. A manual comparison of experimental X-ray diffraction (XRD) peak locations with reference data is usually used to determine phase evolution. The M-type ($MFe_{12}O_{19}$, where M is usually Barium (Ba), Strontium (Sr), or Lead (Pb)) phase evolution in undoped as well as Zinc (Zn) –Zirconium (Zr) co-doped barium hexaferrite samples synthesized using solid state reaction route is investigated in this study using a combination of Pawley and Rietveld analysis. The raw mixed a) undoped and b) Zn-Zr co-doped barium hexaferrite samples were calcined at temperatures ranging from 900 °C–1350 °C for various periods of time (6-12 hours) durations. The structural investigations show that between 1200 °C and 1350 °C, a single M-type phase form (in both undoped and doped samples). Below 1200 °C, the Fe_2O_3 phase in undoped materials and the ZrO_2 and $ZnFe_2O_4$ phases in doped samples have been detected as impurities. In both cases, the structural data was successfully revised using the P63/mmc (number 194) space group.

a0012
Effect of Niobium (Nb^{5+}) Substitution on Dielectric and Piezoelectric properties in ($Na_{0.41}$ $K_{0.09}$ $Bi_{0.5}$) TiO_3 Ceramics
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In the present study, we focused on the dielectric and piezoelectric properties of niobium modified ($Na_{0.41}$ $K_{0.09}$ $Bi_{0.5}$) TiO_3 ceramics which were prepared by conventional solid-state reaction method. The dielectric measurements reveal gradual lowering of depolarization temperature with the increase in niobium content which implies disruption of ferroelectric ordering. The piezoelectric coefficients were found to increase till 0.5 mol% of Nb and for higher doping concentration the coefficients decrease rapidly. The results have been explained on the basis of donor like behavior of Nb doping at lower concentration and for higher doping concentration based on lowering of depolarization temperature.

a0013

Is e/a Ratio The Driving Factor For The Scaling Of Martensitic Transition Temperature In Heusler Alloys?

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Martensitic transition temperature (T_M) generally scales with the average valence electron per atom (e/a) ratio in Ni-Mn Heulser alloys. The e/a ratio can be increased either by increasing Ni content in lieu of Mn or Ga (Ni-rich) or by substituting Mn for Ga (Mn-rich). For the first time a difference between the behavior of Ni-rich and Mn-rich alloys is identified. While both, Ni-rich and Mn-rich Ni-Mn-Ga alloys exhibit martensitic transition, only Mn-rich Ni-Mn-Sn alloys display martensitic behaviour.

a0014

Continued functions and resummation methods

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Few resummation methods are discussed where convergence nature is optimized using continued functions to get precise measures for critical exponents. These simple tools are helpful in handling divergent solutions obtained from perturbative renormalization techniques used in field theories to study continuous phase transitions.

a0015

Quantum Oscillation Signatures in Nodal Line Semimetals under Steady and Oscillating Variation of Magnetic Field

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Quantum oscillation in nodal line semimetals (NLSM) is probed on the basis of spectral calculations in a NLSM continuum model under strong magnetic field. From the Landau level spectra and its evolution with field, we quantify the Fermi level fluctuations. At the same time, the bifurcation of the spectral peaks due to Zeeman splitting and turning of the same due to changes in effective electronic masses are also reported. The direction of magnetic field is an important parameter to the problem and density of states show series of peaks in succession only if the field lies normal to the nodal plane. For magnetic field in the nodal plane, the density of state peaks do not repeat periodically with energy anymore. There one also gets topological oscillations at low energies. Thus properly chosen oscillating field variation can result in topological transitions to occur periodically in these systems.

a0016

Pressure Induced Structural Phase Transition in Tetragonal $BaCu_2(VO_4)_2$: A Raman Spectroscopic and XRD Investigation

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The high pressure structural stability of orthovanadate $BaCu_2(VO_4)_2$ is investigated using in-situ Raman spectroscopy and synchrotron X-ray diffraction up to 26 and 28 GPa respectively. The observations suggest onset of a pressure induced structural phase transition above 18 GPa. X-ray diffraction indicates that the new structure could be lower symmetry crystal structure than tetragonal while the Raman spectroscopic study indicates change in local symmetry around vanadium atom or V-O coordination.

a0017

High Pressure Raman Investigation on Thullium Doped Ceria

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High pressure room temperature Raman investigation on thulium doped ceria ($Ce_{0.8}Tm_{0.2}O_{1.9}$) was carried out up to 24.2 GPa. The ambient fluorite structure (SG: *Fm*3*m*) was observed to remain stable up to 18.8 GPa above which a phase transition was observed. The phase transition was found to be reversible.

a0018

Structural, Electrical and Optical Properties of Lead Free BFO Modified Sodium Potassium Niobate Ceramics

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KNN ($[K_{0.5}Na_{0.5}]NbO_3$) based ceramics are considered to be a very good candidate to replace lead based materials. The system under investigation (1-x) $(K_{0.5}Na_{0.5}]NbO_3$-xBiFeO3 ceramic were prepared using conventional solid state reaction method. The room temperature crystal structure of pure KNN is confirmed as orthorhombic. A well-defined phase boundary between orthorhombic and tetragonal phases is obtained at x=0.01 composition and on further addition of BFO it turns to a pseudocubic phase with slight distortions in tetragonal symmetry. Remnant polarisation P_r has shown an enhanced value of 18.56 $\mu C/cm^2$ for x=0.01. The optical bandgap shifts from 3.3 to 2.7 eV with the addition of BFO in KNN.

a0019

Anomalous behaviour of $CaHfO_3$ at Low Temperatures

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Crystal structure and phase stability of CaHfO3 ceramics prepared by solid state reaction method is investigated till 2K using neutron diffraction. It is found to be stabilized in orthorhombic distorted perovskite ($a^-b^+a^-$, space group Pnma) crystal structure from 2K to 300K. Temperature dependence of volume shows quantum (2 K≤ T≤75 K) and classical (100 K≤ T≤ 300 K) behaviours accompanied by anomalies in spontaneous strain, orthorhombicity and octahedral tilt angle. Temperature dependent lattice parameters along the crystallographic axes <100>, <010> and <001> are found to be anisotropic in nature.

a0020

Phase Formation Study in Residue During Incineration of Combustible Wastes

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Phase transformation study on residual ash samples is presented in this manuscript. Samples are collected from plasma incinerator commissioned at BARC, Mumbai for management of combustible and potentially contaminated radioactive solid wastes. Characterization of end residue is a very important aspect to understand phase changes and reactions happening inside the plasma chamber at high temperature environment. Residues, in the form of ash, rock and glass phases were collected and analysed using EDS and XRD techniques. Elemental composition observed are correlated with respective phases of compounds possible in the residual samples. Phase formation kinetics among ash, rock and glass phases is presented here.

a0021

Structurally Engineered Ferroelectric Phase in Sodium Niobate

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We have structurally engineered ferroelectric phase in NaNbO3 by the application of chemical pressure. In order to explore phase stability of this ferroelectric phase with temperature, we analyzed the temperature dependent powder neutron diffraction data upto cryogenic temperatures. Temperature dependent neutron diffraction patterns do not show appreciable change either in intensity or appearance/disappearance of the observed peaks down to 6 K, ruling out any structural transition in the entire temperature range of 300 K to 6 K. Structural parameters obtained by detailed Rietveld analyses of temperature dependent powder diffraction data show that pseudo cubic cell parameters a_p, b_p and c_p come closer with a monotonic increase in the cell parameters with increasing temperature. The electric polarization has been estimated using a simple ionic model and its value is found to decrease with increasing temperature. Total spontaneous polarization was estimated using refined structural data to be ~ 3.2 μC cm-2 at 6 K.

a0022

Low-Temperature Spin Relaxation Dynamics in Chiral Ferromagnet $Co_{4.5}Fe_{3.5}Zn_8Mn_4$

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We report the spin relaxation dynamics of chiral ferromagnet $Co_{4.5}Fe_{3.5}Zn_8Mn_4$ compound. The compound forms in the cubic chiral space group of $P4_132$. The system undergoes both ferromagnetic and spin-glass like transitions at the temperatures of T_c = 210 K and T_g = 12 K respectively. Study on spin relaxation behavior indicates towards the spin-glassy ground state at $T<T_g$.

a0023

Influence of Fe doping in Structural and Electronic Properties of topological insulator $PbBi_2Te_4$: Experimental & Theoretical Insight from DFT Simulations

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$PbBi_{1.95}Fe_{0.05}Te_4$ was investigated for electronic and structural properties. We have carried out high pressure x-ray diffraction experiments up to 18 GPa. Signatures of structural phase transitions were observed at 7 and 18 GPa. The second, high pressure phase at 18 GPa was determined to be a cubic substitutional alloy phase. Density functional theory predicts that $PbBi_2Te_4$ loses its topological character when doped with Fe and shows conducting bulk states.

a0024

Phase Transition In Selenium Doped Ge-Sb-Te Thin Film For Phase Change Memory

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$Ge_2Sb_2Te_5$ (GST) is extensively studied for phase change random access memory (PCRAM) applications due to its excellent reversible phase transition from amorphous to crystalline phases under high electrical pulses and high switching speed. However, one of the major problems with GST is the high current density required to melt the sample in the SET-RESET transformation. In the present work, GST has been doped with Se, and an increase in the optical band gaps in the amorphous (RESET) and crystalline (SET) states are observed. A significant increase in the SET resistance is also observed in the resistance versus temperature curve which will make it a better candidate for PCRAM.

a0025

High Pressure Raman Spectroscopic Investigation On The Magnetoelectric Material $Co_4Ta_2O_9$

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In recent times, the family of honeycomb antiferromagnets $A_4M_2O_9$ (A = Fe, Co, Mn and B = Nb, Ta) has drawn special attention because of their rich magnetic properties, spin-flop transition and magnetoelectric effect. High pressure investigation on these materials with corundum-type trigonal structure assume significance as pressure-tuning of the crystal structure of these materials can modify magnetoelectric properties. We have synthesized and studied the magnetoelectric material $Co_4Ta_2O_9$ at ambient and high pressures using Raman scattering up to 23 GPa. At ambient pressure, 16 Raman modes have been detected, which are assigned according to the earlier Raman study on the isostructural system $Mn_4Nb_2O_9$. The appearance of two new prominent Raman modes and a few low intensity modes have been observed above 20 GPa, suggesting the onset of a structural transition. Comparing structural transitions in similar structure materials, we speculate the high pressure phase above 20 GPa might be monoclinic.

a0026

Kuramoto Model with Additional Nearest-neighbor Interactions: Existence of a Nonequilibrium Tricritical Point

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The Kuramoto model serves as a paradigmatic framework to study the phenomenon of spontaneous collective synchronization. The usual Kuramoto model involves phase oscillators of distributed natural frequencies interacting via a mean-field interaction. In our present work, we study a variation of the model by including nearest-neighbor interactions on a one-dimensional periodic lattice. For unimodal and symmetric frequency distributions, we show that a competition between the two types of interactions brings in new features, and consequently, the resulting dynamics in the nonequilibrium stationary state exhibits a very rich phase diagram with both continuous and first-order transitions between synchronized and unsynchronized phases, with the transition lines meeting at a tricritical point. Our results are based on numerical integration of the dynamics as well as an approximate theory involving appropriate averaging of fluctuations in the stationary state.

a0027

Spall Fracture in OFHC Copper under Dynamic Loading

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Plate impact experiments were carried out in oxygen free high conductivity (OFHC) copper using single stage light gas gun facility to understand the behaviour of spall fracture strength and yield strength under dynamic loading condition. For each experiment, the rear free surface velocity history was monitored using in-house developed photon Doppler Velocimetry (PDV) and the same exploited to determine the spall strength and dynamic yield strength of this material. Planar shock loading experiments conducted in the velocity range of 260 m/s to 720 m/s evealed that the spall strength of copper varies from 1.06 GPa to 1.21 GPa with corresponding average strain rates ranging from 1.70×10^4 s^{-1} to 3.51×10^4 s^{-1}. This value of spall strength is almost five times more than the quasi-static value of 0.233 GPa(ultimate tensile strength). Similarly, the dynamic yield strength of ~0.24GPa-0.40GPa, is also significantly higher than the static value of 0.218 GPa.

a0028

First Principles Study of Rutile Structure of ThO_2

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ThO_2 is found in fluorite (cubic) structure in nature and is used as nuclear fuel material. At higher pressure, fluorite structure transforms to cotunnite (orthorhombic) structure. These two structures of ThO_2 have been studied extensively. In present work, we have studied the stability and thermo-physical properties of rutile (tetragonal) structure of ThO_2 and compared it with properties of cubic structure. We have used density functional theory (DFT) with spin orbit coupling (SOC) to carry out our work. The optimized lattice parameters of rutile ThO_2 are found as a = c = 5.29 Å and b = 3.75 Å. The absence of negative phonon in phonon dispersion curve shows stability of these structures. Cubic ThO_2 shows higher value of vibrational specific heat and vibrational entropy than rutile ThO_2.

a0029
High Pressure Study of Thorium Dicarbide (ThC_2): An *Ab-initio* Investigation
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Systematic first-principle calculations have been performed to understand the structural stability of thorium di-carbide (ThC_2) under hydrostatic compression using the evolutionary structure search algorithm as implemented in the universal structure predictor: evolutionary Xtallography (USPEX) code in conjunction with ab-initio electronic band structure calculation method. ThC_2 exists in monoclinic crystallographic phase with space group (SG) C2/c. Our calculations under GGA approximation predict the high pressure structural sequence of monoclinic I (SG no. 15, C2/c) $\rightarrow$ monoclinic II (SG no. 12, C2/m) $\rightarrow$ orthorhombic I (SG no. 51, Pmma) $\rightarrow$ orthorhombic II (SG no. 71, Immm)$\rightarrow$ hexagonal (SG no. 191, P6/mmm) for this material with transition pressures of ~ 3.3 GPa, 58.3 GPa, 191.6 GPa and 255.0 GPa, respectively.

a0030
Effect of doping Nb^{5+} in NBBT and study of electrical properties and energy storage performance
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The lead-free ferroelectric energy storage devices of (0.94) $(Na_{0.5}Bi_{0.5})$ TiO_3-(0.06) $BaTiO_3$+ x wt.% Nb^{5+} (x=0%-2.5%) was synthesised by the solid-state reaction technique. The phase has been confirmed by X-ray powder diffraction analysis. The electrical properties of the material were analysed and subsequent energy storage density (W), energy efficiency (η), and energy loss (W_{rec}) were investigated.

a0031
Interplay of Symmetry and Defects during the Topological Phase Transitions
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To investigate the effect of defects on the properties of a topological material, we analyze Kitaev chain with the addition of engineered effective term, in a theoretical way. Here we

analyze the momentum space characteristics like topological invariants, quasi-particle excitation energy, topological quantum critical lines, ground-state energy, and symmetry. We show the behavior of defects and its consequences on the momentum space characteristics of the Kitaev chain. With the appearance of fractional topological invariants, we observe a transformation of system from BDI symmetry class to AIII symmetry class.

a0032

Improved Carrier Mobility of $MAPbBr_3$ Perovskite Crystal Prepared via Low-temperature In-situ Growth Method

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In the current utilization of organic halide perovskites, single crystals show promising properties for optoelectronic applications. The requirement of low trap density and high carrier mobilities with the simple solution grown method is essential for application in semiconductor devices. For this, in-situ, room-temperature assisted synthesis of methylammonium lead bromide ($CH_3NH_3PbBr_3$) crystals using N-methyl formamide (NMF) as a solvent and source of methyl ions during the crystallization process was explored towards understanding the structural, optical, and electronic properties of as-grown crystals. With the approachability of this simple method and also with the improved structural stability, carrier mobility values, the as-grown crystals are useful in photovoltaic applications.

a0033

Influence of Sintering Temperature on Structural and Dielectric Properties of $BaZr_{0.15}Ti_{0.85}O_3$

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In this study, the influence of sintering temperature on the structural and dielectric properties of $Ba(Zr_{0.15}Ti_{0.85})O_3$ is examined. The samples prepared via solid state reaction route were sintered at 1100 ^{0}C and 1300^{0}C. Phase analysis was done by X-ray diffraction. The dielectric properties were analysed over a comprehensive range of frequency and temperature. The analysis of diffraction pattern shows an increase in crystallinity and shift of peaks towards lower diffraction angle. The dielectric constant increase with increase in sintering temperature and dielectric loss has value less than 1.

a0034

Modulational instability of spin-orbit coupled Bose-Einstein condensates with higher-order interaction

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We study the effect of higher-order interaction on the modulational instability (MI) of spin-orbit coupled Bose-Einstein condensates (BECs). The analysis performed for equal densities of the components. Different combinations of the signs of intra- and inter-component interaction strengths are considered. Effects of the two-body interaction, higher-order interaction, Rabi coupling and spin-orbit coupling on the MI of the spin-orbit coupled BECs are investigated, which is not discussed before.

a0035

High Temperature Structural Phase Transitions in Lead-free Piezoelectric $Ba_{0.95}Ca_{0.05}Sn_{0.09}Ti_{0.91}O_3$ Ceramic

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High temperature structural investigations were carried on $Ba_{0.95}Ca_{0.05}Sn_{0.09}Ti_{0.91}O_3$ ceramic powdersynthesized by solid-state reaction method. The line-profile and Rietveld refinement analyses for temperatures ranging from 300K-500K revealed a co-existence of tetragonal, orthorhombic phases at 300K and tetragonal, cubic phases in the range 320-375K. Our results are in correlation with the observed anomalies in the dielectric response.

a0036

Non-Hermitian Topological Quantum Criticality

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Non-Hermitian topological systems are becoming increasingly important in the field of condensed matter because it opens a more realistic and practically possible area to understand the interaction between the system and the environment. We study and present the results of non-Hermitian effect on topological quantum criticality. We use the zero mode solutions (ZMS) to present the topological quantum criticality phase diagram. We observe an interesting feature of multicritical point for the non-Hermitian system. We also present one to one correspondence between the Hermitian and non-Hermitian topological quantum criticality.

a0037

Photoinduced Phase Transitions in Azo doped Cholesteric Liquid Crystal

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In this paper the quantitative comparison of the photo-induced phase transition activity photoresponsive azo dye doped cholesteric liquid crystal was investigated under UV light (365 nm) irradiation with two intensities 2 and 5 mW/cm^2. The conversion of *trans to cis* isomerization of azo molecules caused a shift ΔT upon incident UV irradiation. The dynamic response times are calculated by specifying response times for UV ON and OFF cases in the CLC–I shift region at different temperatures and intensities.

a0038

Temperature-Dependent Raman Studies of Lead-Free $K_{0.5}Na_{0.5}NbO_3$ Piezoelectric Ceramics

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$K_{0.5}Na_{0.5}NbO_3$ (KNN) is well studied due to its excellent electrical, dielectric, ferro, and piezoelectric properties. KNN ceramics have been synthesized by the solid-state reaction method. The X-ray diffraction pattern confirms the orthorhombic phase corresponding to the Amm2 space group. The effect of temperature variation on the Raman spectrum has been studied briefly. The prominent peaks corresponding to υ_1 stretching mode and υ_5 bending vibration modes are related to the internal vibrations of the NbO_6 octahedron. The Raman intensity is enhanced and shifts towards the higher wavenumber at low temperatures. Similarly, there is a Raman shift along the lower wavenumber with a temperature rise. An indication of phase transition has been observed around -80^{o}C and 210^{o}C because of spectral change and corresponding shifts.

a0039

Synthesis of Nano Silicon Carbide by Reaction Conversion Method

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Carbon soot was successfully converted into silicon carbide by reacting with SiO vapour at 1500˚C under Ar gas environment at atmospheric pressure. The holding time for reaction and flow rate of Ar gas were varied ranging between 6-20h and 50-250 ml/min, respectively. The structural and microstructural property of synthesized SiC were characterized using X-ray diffraction (XRD), Raman spectroscopy and scanning electron microscopy (SEM). Carbon residues were removed by heating it over 750˚C for 6h. It has been observed that final yield and phase structure of synthesized SiC is dependent on reaction holding time and Ar gas flow rate.

a0040

Fascinating phase evolution in the x $Na_{0.5}Bi_{0.5}TiO_3$- (1-x) $NaNbO_3$ lead free binary solid solutions

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The structural studies of lead free solid solutions x $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) – (1-x) $NaNbO_3$ (NN) for $0 \leq x \leq 1$ is done using X-ray diffraction. The appearance/disappearance of the super lattice reflections along with the change in the intensities of the main cubic perovskite peaks in diffraction data provides clear evidence for structural phase transitions with composition. The Detailed Rietveld refinements revealed that these solid solutions systematically undergo structural phase transitions from the room temperature AFE (*Pbcm*) phase of pure NN to FE (*R3c*) phase of pure NBT through different phases. Initially the AFE orthorhombic (*Pbcm*) to ferroelectric ($Pmc2_1$) at x>0.05 then FE orthorhombic ($Pmc2_1$) to Paraelectric (PE) (*Pbnm*) at x> 0.20 after that PE Orthorhombic (*Pbnm*) to AFE (*P4bm*) at x>0.70 finally to AFE Tetragonal (*P4bm*) to FE Rhombohedral (*R3c*) at x> 0.80. The dielectric measurements at room temperature recorded also shows the anomalies with composition.

a0042

Temperature Dependent Crystal Structure Of $CaCeTi_2O_7$

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Herein the evolution of crystal structure of pyrochlore type $CaCeTi_2O_7$ in between 50 to 1273K is reported from low temperature powder neutron diffraction and high temperature powder X-ray diffraction studies. The Ca and Ce is statistically occupied in the A site of pyrochlore lattice forming distorted eight coordinated polyhedra while the Ti atoms are occupied in the B sites forming regular octahedra. Besides, the powder neutron diffraction studies revealed no detectable oxygen vacancies, suggesting that all the Ce atoms are in 4+ oxidation state. The unit cell parameter shows a smooth variation with increasing temperature, and the coefficient of volume thermal expansion in between 50 to 1273 K is 32.6×10^{-6} K^{-1}.

a0043

Modulational instability of spin-orbit coupled Bose-Einstein condensates with two- and three-body interactions

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We study the modulational instability of spin-orbit coupled Bose-Einstein condensates with two- and three-body interactions (TBIs). The analysis performed for equal densities of the components. Different combinations of the signs of intra- and inter-component interaction strengths are considered. Effects of the two-body interaction, TBI, Rabi coupling and spin-orbit coupling on the modulational instability of the spin-orbit coupled Bose-Einstein condensates are investigated, which is not studied before.

b: SOFT CONDENSED MATTER INCLUDING BIOLOGICAL SYSTEMS

b0001

pH Dependent Structural Evolution of Plant NanoFibrillar-Network During Dehydration: Real time SAXS investigation

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Dehydration driven structural shrinkage of fibrillar network is an important and ubiquitous phenomenon in nature. We have used time-resolved small-angle X-ray scattering (SAXS) to get the insight into such structural modification. Temporal evolution of shrinkage of inter-fibrillary voids is found to be strongly dependent on the nature of hydration medium. For neutral and acidic media, temporal shrinkage follows a logistic model but shrinkage in case of alkaline medium remains insignificant. For neutral and acidic media, the Porod level, an indicator of contrast weighted volume fraction, exhibits a maximum. However, a contrasting behaviour is observed for alkaline medium. Scanning electron microscopy and infrared spectroscopy reveal significant alteration of fibrils under hydration in strong alkaline medium.

b0003

A Spectroscopic Ellipsometric Study of PVDF/PEG Polymer Blends

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Polymer blends (*PB**)*** comprised of polyvinylidene fluoride (PVDF)/ polyethylene glycol (PEG) were synthesized in the form of thin films through the two step solution casting method. The optical properties of the ***PB*** were studied through spectroscopic ellipsometric study in the visible region of wavelength (500 nm -800nm). The various optical constants (e.g. refractive index, extinction co-efficient, etc.) & their dispersion behavior over the visible range of wavelengths show large variation as a function of compositions due to the different extent of interaction of matrix/filler. The optimized parameters were obtained for the 20% PB sample suggesting the sample to be a better material, suitable for various optical applications.

b0005

Distribution of Non-ionic Micelles Adsorption on Different Sized Silica Nanoparticles

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The adsorption of non-ionic surfactant C12E10 micelles on two different sizes of anionic silica nanoparticles (16 and 27 nm) has been studied by small-angle neutron scattering. The number of adsorbed micelles per nanoparticle strongly depends on nanoparticle curvature and increases with nanoparticle size, as a result, their surface density increases but the fraction of adsorbed micelles decreases with increase in nanoparticle size. In a bimodal system of these nanoparticles, three possibilities of micelles adsorption are examined (i) preference for larger sized nanoparticles, (iii) preference for smaller sized nanoparticles and (iii) no preference for any size. The results support to the non-preferential adsorption of micelles on different sized nanoparticles.

b0006

Resonator-based, Functionalized Biosensor for Diagnostics of Dengue NS1 Antigen

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A non-invasive microwave-based complementary split-ring resonator (CSRR) sensor is proposed to detect the dengue NS1 antigen. The CSRR antenna structure is etched out of copper, on the ground plane of a micro strip line using a printed circuit board (PCB) technology on the FR4 substrate. The micro-strip transmission line coupled with CSRR acts as a sensor whose sensing mechanism is based on the interception of the electromagnetic field around the resonator, which leads to a shift in the resonance frequency. To detect dengue NS1 antigen, the sensor is functionalized with the antibody of NS1 using 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (EDC) as the linker molecule. Upon immobilizing NS1 antibody on the CSRR structure, the sensor offers high sensitivity in the form of a change in the power of the signal due to antigen-antibody interaction. The sensor shows a power shift of ~24dB for 10 µl of dengue NS1 antigen. A highly sensitive sensor is hence demonstrated.

b0007

Host-parasite coevolution: Role of spatial topography of fitness landscape on evolvability of hosts

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We study a mathematical model which describes the host-parasite coevolution in a fluctuating environment by incorporating mutation, selection, and asexual reproduction. The role of spatial topography of the fitness landscape on the evolutionary dynamics of a finite population of hosts is investigated. We report the dependence of time required by the host population to attain the global maximum of the fitness landscape on the ratio of the global and local fitness peak heights for different host mutation rates and different degrees of virulence. We find a faster optimization of hosts' fitness and a reduced dependence of optimization time on the degree of parasitic infection in case of a higher disparity between the global and the local fitness peaks.

b0009

Effects of L-Phenylalanine on a Model Phospholipid Membrane

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Biological cell membranes play a crucial role in controlling the physiological activities of various chemical components in a living organism. Despite of various roles that include causing diseases in humans, the effect of phenylalanine (Phe) on cellular membrane is still not clear. In this work, the physical and structural changes in a model cellular membrane in the presence of L-Phe have been investigated using surface pressure-area isotherms and X-ray reflectivity technique.

b0010

Experimental Investigation of Phases Of Different Lattice Structures Of Surfactants-DNA Complexes

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Small angle X-ray scattering (SAXS) technique reveals the structures of surfactants-DNA complexes, which acquires hexagonal phase in presence DTAB and MTAB in aqueous media for both relative concentration ratios, ([MTAB] + [DTAB])/[DNA]= ρ), 1 and 5. Structures undergo a phase transition due to an influence of NaCl salt. The structures enter a super hexagonal phase in presence of a large amount of DTAB (wt %) in 300 mM NaCl solutions for ρ 1. The structures gradually obtain a square phase for increasing the amount of DTAB (wt %) in 300 mM NaCl solutions with ρ 5.

b0011

Water Desorption Kinetics Of Poly(vinyl alcohol) Thin Films

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The water desorption kinetics in one-dimensional confined PVA thin films has been studied using temperature-dependent spectroscopic ellipsometry (SE) and in bulk PVA through thermogravimetric analysis (TGA). Two characteristic temperatures, T_{C1} and T_{C2} are identified that distinguish three different processes of desorption of unbound free water, thermal expansion, and desorption of tightly bound water that the film undergoes during its first heating. Interestingly, for the thinner film of 39 nm thickness, the magnitude of such thermal expansion becomes even more prominent in comparison to the 72 nm film. Further, through TGA, the presence of different phases of water desorption (three regions) has been confirmed and their corresponding activation energies are estimated.

b0012

CO_2 Adsorption-Desorption Kinetics on Silica-Polyethyleneimine Microspheres obtained through Evaporation Induced Assembly

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In the current scenario of global warming, mitigation of CO_2 remains a challenge to tackle with. However, amine-based solid adsorbents have provided a potential way to surmount this facet. In order to revamp the performance and design of CO_2 capture reactors study of adsorption/desorption kinetics is crucial. Such kinetics on microspheres with 20% amine loading is studied using thermo-gravimetric analysis at different temperatures under CO_2 flow. The kinetics of adsorption follows Avirami model, whereas desorption kinetics resembles to dose-response model for low adsorption temperatures and approaches exponential decay model at higher temperatures. Higher temperature results in homogeneous adsorption due to sufficient kinetic energy of CO_2 molecules and better accessibility of amine sites, which sequentially increases the sorption capacity.

b0013

Recrystallization of Poly(vinylidene fluoride) Membrane: Enhancement In The Spherulite Morphology

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We report the temperature-dependent spherulitic growth and microstructural evolution of the non-crystallized and crystallized Poly (vinylidene fluoride) (PVDF) membranes. The recrystallization of the α-phase PVDF membrane leads to the formation of prominent spherulites and its reversibility is confirmed using in-situ temperature-dependent x-ray diffraction. Temperature dependent in-situ optical microscopy revealed that the nucleation and growth of spherulites start at a higher temperature for alpha-PVDF and results in spherulites of much larger size during the recrystallization process.

b0014

Water Vapor Triggered Rapid Actuation of Cotton Films

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Stimuli-responsive soft actuators are gaining much research attention in recent years and remain a rapidly growing field with many applications. Here, we report the fully reversible and repeatable actuation characteristics of free-standing cotton films upon exposure to water vapor. Cotton has added advantage of being biopolymers that are biodegradable and sustainable. A minuscule quantity of water vapor is sufficient to generate significant macroscopic responses. The differential swelling-induced anisotropic strain generated across the thickness of the cotton film is the driving force responsible for the observed actuation characteristics.

b0015

Phase Transition In An Implicit Solvent Minimal Model Of Lipids: Role Of Head-Tail Size Ratio

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We present Monte Carlo simulations under constant NVT conditions on a minimal 'three beads' coarse grained implicit solvent model of lipid molecules, with the hydrophilic head represented by one bead and the hydrophobic tail represented by two beads. We consider two lipids, one with the head and tail bead sizes equal and the other with the tail beads smaller than the head. When cooled to the ambient temperature from an initial isotropic phase at high temperature, the first lipid transforms spontaneously to a lamellar phase while the second lipid transforms to a micellar phase, showing the crucial role of the head-tail size ratio on lipid phases.

b0017

Charged Active Particle in the Presence of Magnetic Field

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We consider the dynamics of a charged inertial active particle self-propelling in a 2D harmonic trap. The dynamics is further subjected to the presence of a magnetic field applied perpendicular to the plane of its motion. The particle is modeled as an active Ornstein-Uhlenbeck particle (AOUP) with exponentially correlated noise. We have exactly calculated both the position and velocity correlations and investigated the dynamical behavior in various time scales of the dynamics. The analytical results are in good agreement with the simulation and the inertia is found to have significant impact on dynamics. The influence of magnetic field on position and velocity correlation persists only in the inertial regime of the dynamics and disappears for highly viscous medium.

b0018

Dynamical Heterogeneity in Deep Eutectic Solvents

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The quest for a green solvent media in various industrial processes has been a hot pursuit. Deep eutectic solvents (DESs) are one of the recent additions to this repository. The transport properties of these solvents play a decisive role in their applications. At the microscopic level, they exhibit strong heterogeneity in their dynamics owing to extensive hydrogen bond interactions. In this study, we employ neutron scattering technique to explore the dynamical heterogeneity in acetamide + lithium salt based DESs. The extent of heterogeneity is characterized by deviation from the Gaussian nature of the diffusive dynamics in the system. Among the different salts used, it is found that lithium perchlorate is the least heterogenous and lithium bromide the most.

b0020

Structural Investigation of Quantum Dots Mixed Lipid Membranes

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Use of quantum dots (QDs) instead of organic dyes for the biological application has several advantages. Here we report the Langmuir monolayer studies of phospholipids mixed with QDs to determine the assembly and the bio-conjugation of the QDs
in the membrane. The x-ray reflectivity and AFM studies of the mixed phase monolayer, transferred on to the solid substrate
by inverted Langmuir−Schaefer reveal the lipid head group specific attachment mechanism of QDs with the lipid membrane.

b0021

Observation of Spherical to Non-spherical Transition of Micelles by Different Means

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The non-ionic surfactantC12E10in aqueous solution self-assembles to form core-shell spherical micelles. Different means (temperature, salts and alcohols) have been examined to induce spherical to non-spherical transition of micelles using small-angle neutron scattering (SANS). The dehydration from micellar shell leads to spherical to non-spherical transition in the cases of increasing temperature and selecting salt (e.g. KF). On the other hand for

alcohols, spherical to non-spherical micellar transition arises for long chain length alcohols CnOH (n> 5) because of the mixed micelles formation of alcohol with surfactant. The structural parameters of micelles have been determined from the form factor SANS analysis.

b0022

Modifying Heat-Induced Protein Gelation by Addition of Tetravalent Counter-Ions

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Proteins are known to undergo unfolding on heating due to disruption of the hydrogen as well as disulphide bonds and exposure of hydrophobic groups. This results into the hydrophobic attraction driven gelation of the proteins at significantly high temperatures. We show that the gelation of the protein can be restricted by modifying inter and intra-protein interactions through addition of tetravalent (Zr^{+4}) counter-ions. In the absence of any counter-ions, bovine serum albumin (BSA) protein solution (5wt%, pH ~ 4) transforms into gel, at about 70°, keeping for nearly 2 hours. On the contrary, the BSA solution in the presence of Zr^{+4} does not gel even on heating up to higher temperatures and longer times. Such effect has not been observed to be arising for mono and divalent ions and believed to be originating due to ion-ion correlations, strongly prevailing in case of multivalent ions.

b0023

Biopolymer based Sodium ion Conducting Ecofriendly Electrolyte for Electrochemical Energy storage Applications: Ionic Conductivity and CV Analysis

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A new series of sodium ion conducting biopolymer electrolyte were prepared using solution casting technique. I – Carrageenan and sodium bromide were used as biopolymer matrix, an electrolyte respectively. Both the concentrations of I – carrageenan and sodium bromide were varied. AC impedance spectroscopy result showed that the system with I – carrageenan (0.5 wt%)/sodium bromide (0.5 wt%) exhibited a maximum ionic conductivity of 4.4567 x 10^{-4} Scm^{-1} at room temperature. From CV analysis, the cyclic stability of the high ionic conducting sample was found to be good.

b0024

Surfactant Induced Stabilization of AOT/Water/Dodecane Nano Emulsion Droplet

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SANS measurements have been used to investigate and tune the structure and inter droplet interactions of AOT/Water/dodecane nanoemulsions droplets under varying macromolecular environment around the droplets. The macromolecular environment around droplets was effectively controlled using nonionic surfactant (C12E10), anionic sodium dodecyl sulfate (SDS) and cationic dodecyl trimethyl ammonium bromide (DTAB) surfactants.

b0025

AFM and Variable Range Hopping Conductivity Studies of Silver Sulfide Filled PVA-PEG Polymer Hybrid Material

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Polymer hybrid films were synthesized by solution casting method, using polyvinyl alcohol-polyethylene glycol (PVA-PEG) polymer blend as the organic host matrix, while the inorganic component, silver sulfide (Ag_2S), was prepared in situ in the polymer blend matrix in the absence of sunlight. Surface morphology of the prepared hybrid films was investigated using atomic force microscopy (AFM) technique. Highest value of average surface roughness (S_a) of 62.50 nm was seen for the hybrid film with Ag_2S particles in their micro form. Temperature dependent direct current (DC) electrical measurements were carried out using two probes setup and the data was analyzed using Greave's three dimensional (3D) variable range hopping (VRH) model. Pure polymer blend film has got the highest values of range of hopping (R_{hop}) and hopping energy (W_{hop}).

b0028

Ionic Surfactant-induced Tuning of Block Copolymer Self-assembly

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The role of anionic surfactant sodium dodecyl sulfate (SDS) on the self-assembly behavior of poly(ethylene oxide)-poly(propylene oxide-poly(ethylene oxide) PEO-PPO-PEO triblock copolymer [P85 ($EO_{26}PO_{39}EO_{26}$)] in aqueous solution as a function of temperature has been studied using small-angle neutron scattering (SANS). The measurements have been carried out for fixed concentrations (1 wt%) of block copolymer and surfactant. Each of the individual components (block copolymer and surfactant) and the block copolymer–surfactant mixed system has been examined at varying temperatures. The block copolymer P85 remains as unimer at lower temperature, forms spherical micelles at room temperature whereas shows sphere-to-rod like micelle transition at higher temperatures. On the other hand, surfactant SDS forms ellipsoidal micelles over a wide temperature range. Interestingly, it is found that phase behavior of mixed micellar system (P85 + SDS) as a function of temperature is drastically different than that of the rich phase behavior of P85, giving the control over the temperature-dependent structural transition of block copolymers.

b0031

Preferential binding of ionic surfactant in protein-ionic-nonionic surfactants complex and the resultant structure

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Proteins are known to interact electrostatically as well as hydrophobically with ionic surfactants and undergo unfolding, whereas they show weak interaction with nonionic surfactants. However, the nonionic surfactants bind hydrophobically to ionic surfactants, resulting in the formation of mixed surfactant micelles in the aqueous solution. In the present work, we have investigated the preferential binding of an ionic surfactant [sodium dodecyl sulfate (SDS)] in the protein [bovine serum albumin (BSA)]-ionic-nonionic surfactants [polyoxyethylene 10 lauryl ether (C12E10)] ternary system using Small-angle neutron scattering (SANS). It has been demonstrated the preferential binding of SDS strongly depends on the nonionic-to-ionic surfactant molar ratio. At lower ratios, the strong electrostatic interaction and co-operative binding between the BSA and SDS, leading to the formation of the beads-on-a-string-like complexes with the co-existence of individual

C12E10 micelles. On the other hand, at higher ratios, the hydrophobic interaction of SDS-C12E10 overcomes the interaction between BSA-SDS, leading to the formation of mixed ionic-nonionic surfactant micelles co-existing with the native protein.

b0034

Computer Simulation Study on Polar Biaxial Liquid Crystal Phases

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Computer simulation study on a system of polar biaxial ellipsoid particles is performed. Dipole-dipole interaction is taken as polar interaction along with a new kind of elliptic contact potential (ECP) interaction acting between the molecules. Generation of different polar biaxial liquid crystal phases depending on the temperature are reported.

b0036

Phase Behaviour of Dihexadecyldimethylammonium Bromide Bilayer

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Dihexadecyldimethylammonium bromide (DHDAB) lipids form bilayer in aqueous media exhibiting a rich phase behaviour. In this work, by using Differential scanning calorimetry (DSC) and Fourier transform infrared (FTIR) spectroscopy, we have characterised the phase behaviour of DHDAB bilayer. It is found that in the heating cycle, the system goes from coagel to fluid phase via an intermediate phase. However, the intermediate phase is not observed in the cooling cycle, as the system goes back from fluid to coagel phase directly. DHDAB results have shown very contrast to dioctadecyldimethylammonium bromide (DODAB) bilayer which differs only in the tail length.

b0037

A Quantum Mechanical Prediction Of C_{24} Fullerene As A Biosensor For Adenine Nucleobase

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In this work, we have explored the potential of C_{24} fullerene for the applicability of adenine sensing using density functional theory. Among the different orientations, P1 site found to be minimum energetic configuration. The adsorption energies, interactions distances, NBO analysis, dipole moments and DOS are calculated to understand the impacts of adenine adsorption over C_{24} fullerene. The adsorption energy is -1.16 eV of adenine adsorption over C_{24} with P1 geometry. Our results indicate suitability of C_{24} fullerene in bio-sensing of the adenine molecule.

b0039

Position and Velocity Correlation of Inertial Self Propelled Particle

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We have studied the dynamics of an inertial active particle moving in a solvent with active Ornstein Uhlenbeck process. We have exactly solved the dynamics and calculated the position and velocity correlation functions for the case when the particle is freely propelling as well as when it is confined in a harmonic trap. When the self propelling time is of the order of the inertial delay time of the freely self propelling particle, the velocity at two different times are decorrelated. The correlation corresponding to the deviation in position is the athermal contribution and depends on the activity of the self propelled particle.

b0040

Structural Reorientations and Stability of Curcumin-Chitosan Drug Formulations Embedded to Silica Nanoparticles

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Efficient drug delivery formulations to address low solubility, bioavailability and hence sustained release applications of Curcumin (yellow bioactive component of turmeric), a potential anti-cancer, anti-viral drug, merit detailed structural investigations. Here, curcumin, hydrogen bonded to the polymer chitosan, a well known drug delivery vehicle was encapsulated in microspheres formed by the scaffolds of silica nanoparticles under varying chemical environments, and investigated using infrared spectroscopy at ambient and *in-situ* high temperature conditions. Noticeable spectroscopic features have been shown which highlight the subtle molecular reorientations under varying chemical environments that eventually dictate the structural assembly. The microspheres are found to show good stability upon heating upto 60^{o}C.

b0041

Effect of low dose 200 keV N^+ ion beam irradiation on dielectric and polarization properties of free-standing, flexible films of PVDF-HFP

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Dielectric studies and polarization studies were carried out on low dose N^+ (200 keV) ion beam irradiated free-standing, flexible films of Poly(vinylidene fluoride-hexafluoropropylene) (PVDF-HFP). Effect of the irradiation on the physical properties of the films were studied using Field Emission Scanning Electron Microscopy, X-Ray Diffraction, Raman, and Fourier-transformed infrared spectroscopic studies. The dielectric constant of the pristine films was found to reduce to ~16 from ~21 while the remanent polarisation

reduced to 3×10^{-4} μC/cm^2 from 4.8×10^{-3} μC/cm^2, upon irradiate ion with a dose of 5×10^{12} ions/cm^2 N^+ ions.

c: NANO-MATERIALS

c0001

Surfactant dependent interaction of aminoglycoside antibiotic with metal nanoparticles

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Silver and gold nanoparticles were synthesized by chemical method in the presence of different surfactants. Trisodium citrate was used to study its role as a binder between metal nanoparticles (AgNPs and AuNPs) and aminoglycoside antibiotic named amikacin. Analytical techniques such as UV-Visible absorption spectroscopy, and X-ray diffraction have been used to investigate the interaction mechanism between drug and nanoparticles surface. It has been observed that in case of AgNPs, citrate is not a good linker for amikacin to bind with nanoparticle surface as silver lost its SPR after the addition of amikacin due to formation of unstable sulphur compounds. However, in case of AuNPs, citrate could be used as a linker between drug and nanoparticle surface.

c0002

Gamma Ray Induced on Synthesis of SF-AgNPs: Characterization

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In this work *Bombyx mori* silk fibroin (SF) films were prepared by solution casting method. Gamma irradiation of protein biopolymer films were carried out in dry air at room temperature using Co – 60 source, and radiation doses are in the range of 0-60 kGy. The unirradiated and irradiated films were characterized by the resultant products have been confirmed to be Ag-NPs was carried out based on UV-Vis spectroscopy (427 nm). The UV-visible spectra showed that the characteristic surface plasmon resonance (SPR) band at around 424 nm and high-resolution transmission electron microscopic (HR-TEM) measurements. From this study, it was found that the increasing the radiation dose increases the rate of reduction and decreases the particle size. The size of the AgNPs can be tuned by controlling the radiation dose.

c0004

Nonlinear refraction and absorption in semiconductor core-shell quantum dots

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We present the results of the numerical analysis of the theoretical formulations to examine the occurrence of optical nutation in semiconductor quantum dot of GaAs/AlGaAs subjected to ultra-fast pulsed coherent radiation. The transient values of and enables one to analyze both nonlinear refraction and nonlinear absorption in the quantum dots. The transient nonlinear optical responses have been over a wide range of photon energy for strongly confined excitonic features of the QDs.

c0005

Evidence of Giant Magnetic Moment Clusters and their Disintegration into Small Clusters in a Cobalt Carbide Nanocomposite

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We study the magnetic properties of cobalt carbide nanocomposite with a mixture of Co_2C and Co_3C phases in a 1:1 ratio (volume). *M-H* hysteresis measurements ascertain the presence of significant hysteresis up to room temperature (*T*). Using a modified Langevin analysis of *M*(*H*) curves, we observe that at room temperature, the nanocomposite behaves as a collection of giant magnetized clusters, with each cluster possessing a large average magnetic moment of ~ 4200's μ_B. Each cluster comprising a few hundred Co_3C molecules behave as a single unit exhibiting a giant moment. At high *T*, there are small numbers of these large-sized magnetized clusters. Below 100 K, the number of clusters increases significantly while the size of each cluster decreases, and the average moment per cluster also decreases rapidly down to 30 μ_B. Thus, it appears that there is a fine-graining disintegration transition of these clusters around 100 K. We explain our results by considering that the nanocomposite with clusters possesses a mixture of Co_3C-Co_2C, interspersed with primarily Co_2C rich regions. The strong exchange coupling is mediated within the heterogeneous clusters through free electrons at high *T*, leading to a giant moment. The exchange coupling in these clusters weakens below 100 K leading to the fine graining transition.

c0006

Synthesis and characterization of Spherical shaped silver nanoparticles from extremophilic bacterium *Deinococcus radiodurans*

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In Nanotechnology, the biosynthesis of metal nanoparticles has potential applications in many fields. The particle synthesis from Extra cellular substances of bacterial cells have low cost and eco - friendly, while it can produce with controlling parameters like pH, biomass and growth phase. The extremophile bacteria *Deinococcus radiodurans* that possesses the power to resist very high radiation and desiccation stress has been utilized for the synthesis of silver nanoparticles (AgNPs) during this study. Since it's having distinctive size-dependent properties, silver nanoparticles offer the chance to develop new therapeutics. This work is aimed to synthesis AgNPs from the cell free extract of *Deinococcus radiodurans* and also the silver nanoparticles confirmed through UV-Visible spectrometry, FT-IR, DLS, SEM - EDAX.

c0007

Facile Synthesis of *Terminalia chebula* and *Strychnos potatoram* mediated Titanium Dioxide (TiO_2) Nanoparticle and Its Nano bio application: Comparative study

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Recently there has been increasing interest in developing potent non-toxic drugs in medicine which is widening the chances for studying the usage of nanostructures in nanomedicine. The present work reports a method for a facile and an eco-friendly synthesis of titanium di oxide nanoparticles (TiO_2 NPs) using *Terminalia chebula* fruit extract (TCE) and *Strychnos*

potatoram. In the selection of herbal scenario for current usage, *Terminalia chebula* (Kadukkai) and *Strychnos potatoram* (Thettan Kottai), are the oldest herbal medicinal plant which is called as the King of the Medicine's, and they contain a number of chemical constituents like chebulic, ellagic acid, tannic acid, alkaloids, flavonoids', saponins, etc. Hence the main aim of this work is to facile synthesis of TiO_2 NPs from the aqueous extract of *Terminalia chebula* and *Strychnos potatoram*. The obtained Titanium Dioxide nanoparticle has been characterized by UV Visible Spectrophotometer, Fourier Transforms Infra-Red Spectrophotometer, SEM, Dynamic light scattering and Zetapotential. In addition, a comparative study of its antioxidant activity was analysed.

c0008

Fluorescence Emission Enhancement Of Copper Nanoclusters (CuNCs) In The Presence Of Ascorbic Acid

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An environment friendly chemical synthesis method is used to synthesize lysozyme templated ultra-small copper nanoclusters (CuNCs). The as-synthesized NCs shows an UV-Vis absorption around 365 nm and an emission at around 449 nm corresponding to this absorption. The fluorescence emission of CuNCs enhances with increasing concentration of ascorbic acid. The interaction of surface lysozyme with ascorbic acid may be the reason behind such enhancement. Due to interaction, the NCs possibly form aggregates and the aggregation induced enhancement in emission is observed.

c0011

Impact of Thermal Treatment on Surface Morphology and Band Gap Modification of In_2O_3/SiO_2 Nanocomposite

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In the present study, we have demonstrated the impact of thermal treatment on surface morphology and band gap modification of In_2O_3/SiO_2 nanocomposite using sol-gel technique. The powder samples are calcined at various temperatures those are further examined by famous characterization tools. The cubic phase of prepared sample is confirmed by XRD and microstructure details are obtained from SEM study. The surface interactions play a crucial role in determining the morphology and crystal phase which further modify the band gap of prepared In_2O_3/SiO_2 nanocomposite.

c0014

Optical, AC conductivity and dielectric properties of pure and Ag doped TiO_2NPs prepared by microwave assisted synthesis method

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Pure Titanium oxide (TiO_2) and Ag doped (0.04 mol%) nanoparticles (NPs) were prepared by microwave-assisted method, and were characterized by XRD, UV-visible spectroscopy, and dielectric techniques. XRD patterns of both samples suggested the presence of anatase tetragonal structure. Rietveld refinements on XRD plots of both samples by GSAS package

confirmed the proper incorporation of Ag at TiO_2 lattice by showing significant variation between lattice parameters of pure and Ag doped TiO_2 nanoparticles. UV–Vis spectroscopy results confirmed the presence of direct band gap in both the samples; however Ag doping reduces the optical band gap but increases Urbach energy, which is the clear indication of red shift in Ag doped TiO_2 NPs. So, these defect states are increased by Ag doping in TiO_2 NPs system. The dielectric measurements showed that the dielectric constant increased as frequency of applied field increases. The conductivity of both samples followed Jonscher's power law. The non linear least square fittings on Nyquist plots of both samples suggested that conduction process took place predominantly through grain boundary in both samples; however, influence of grain boundary in Ag-TiO_2 NPs is reduced. These results were discussed by correlating optical and dielectric properties of TiO_2 and Ag doped TiO_2 NPs which gave broad understanding to device fabrications successfully.

c0015

Transport and Optical Properties Of Selenium Rich $MoSe_2$ Nanospheres

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In this work, we investigated the transport and optical properties of Molybdenum diselenide ($MoSe_2$) nanospheres synthesized using hydrothermal technique. Temperature dependent resistance measurement revealed two conduction regimes, one dominated by degenerate electrons contributed by excess Se and the other by phonons and impurities. The transport regime dominated by degenerate electron was observed from 300 to 70 K, with conductivity decreasing with decrease in temperature. From the Arrhenius plot, the activation energy for the electrons is found to be ~0.5 meV which is the activation energy for the electrons from uncompensated Se atoms. In the low temperature regime (below 70 K) the nanosphere exhibited a metallic like behavior with conductivity increasing with decrease in temperature indicating that the electron transport is dominated by impurities and phonons. Our findings revealed that hydrothermally synthesized $MoSe_2$ is Se rich and has the characteristics of a degenerate semiconductor.

c0016

Efficient Broad-Spectrum UV attenuation By Defect Engineered ZnO Nanodots Synthesized By A Facile Wet Chemical Batch Process

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Defect engineered ZnO nanodots (E-NDs) exhibiting high quantum yield with efficient UV attenuation were synthesized by a novel facile wet chemical approach in a batch reactor with enhanced reaction kinetics. This synergistic effect of fast nucleation-growth facilitates the enrichment of singly ionized oxygen vacancy defects (Vo). The E-NDs exhibited high photostability with long-lasting photoluminescence, narrow particle size distribution of its stable dispersion and superior radical scavenging characteristics.

c0018

Structural and Colloidal Stability Studies Of PVA Functionalized Greigite

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The magnetic nanoparticles (MNPs) have been intensively studied due to their wide range of applications such as magnetic bioseparation, drug delivery, and magnetic hyperthermia for cancer therapy. Hyperthermia, which uses magnetic nanomaterials with high heating efficiency, is a promising alternative for the conventional modalities of cancer treatment. The functionalization of MNPs is crucial as it increases chemical stability and biocompatibility and reduces toxicity. Superparamagnetic Iron Oxide Nanoparticles (SPIONs) have been thoroughly investigated and dominated Magnetic Hyperthermia and demands researchers to explore other magnetic materials. Greigite (Fe_3S_4), a ferrimagnetic iron sulfide mineral analogous to magnetite with an inverse spinel structure, is least studied for magnetic hyperthermia. The present work is about synthesizing Greigite nanoparticles by solvothermal method and its surface functionalization by the amorphous polymer PVA. The XRD analysis reveals the formation of the Greigite and the presence of PVA coating on the surface of the nanoparticles. The average particle size from FESEM analysis for the uncoated and PVA coated samples are 11.626 nm and 62.487 nm, respectively. The functional groups identified from FTIR spectra indicate the presence of PVA layer on the surface of PVA coated greigite nanoparticles. The increased hydrodynamic size for the coated sample confirms the PVA coating on its surface, and its higher zeta potential compared to the uncoated one indicates that PVA can enhance the colloidal stability of Greigite.

c0019

Heat-Induced Silver Nanoparticles Inside Poly(vinyl alcohol) Film

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Poly(vinyl alcohol) (PVA)-silver (Ag) nanocomposite films are prepared for different heating periods and their structure, optical and mechanical properties are investigated. UV-visible absorption spectrum shows localized surface plasmon resonance peak at around 433 nm due to the formation of silver nanoparticles. XRD spectrum also indicates the incorporation of silver salt inside PVA matrix. The size of the spherical silver nanoparticles formed inside PVA-Ag composite film heated for 15 min is obtained as 26.3 ± 0.6 nm. Loading-unloading test shows decreasing hysteresis loop area with increasing the number of cycle.

c0020

Non-Linear Optical Properties of PMMA Doped ZnO Thin Film

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In the present work, ZnO nanoparticles were synthesized using sol gel method. Polymethyl methacrylate (PMMA) doped ZnO thin film was casted by drop-casting method. Using XRD the average grain size found to be 34 nm. To study the bonding nature of the ZnO nanoparticles FTIR study was done. The linear optical properties were studied by UV-Visible spectra. Nonlinear absorption of prepared thin film was examined using open aperture z-scan

technique at different intensities. We found that the nonlinear absorption coefficient (β) decreases on increasing the intensity.

c0021

Formaldehyde Gas Sensing Properties of Hafnium Oxide Nanopowders Synthesized by Sol-Gel Method

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This work reports the development of an interesting chemiresistive formaldehyde gas sensor based on hafnia (HfO_2) nano-powder. Monoclinic HfO_2 nano-crystals were synthesized by sol-gel route at two different calcination temperature viz. 500 ºC and 700 ºC. The gas sensing characteristics of HfO_2 were studied by employing formaldehyde gas at four different concentrations ranging from 1000 to 30000 ppm. HfO_2 sensor shows high response under formaldehyde exposure. Also, the shorter reaction and recovery time and linear response suggest that HfO_2 could have a potential application in formaldehyde gas sensor fabrication.

c0023

Analysis of Cinnamon Zeylanicum Bark Extract Infused Nickel Oxide Nanoparticles as Efficient Drug Delivering Agent

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Nickel Oxide Nanoparticles takes a special place and interest for its various application in optoelectronics, magnetism, catalysis, solar cells, sensors and many other environmental and biological applications Because of their exceptional properties, these NiO nanoparticles are being studied extensively. Antiferromagnetism is another significant strategic property of NiO nanoparticles, which leads to increased biosystems applications. The bark of Cinnamon. zeylanicum has been shown to have impressive pharmacological effects in the treatment of type 2 diabetes and insulin resistance. With regard to biomaterial dosage and pH, we have discussed the drug delivering efficiency of NiO nanoparticles using C. zeylanicum bark powder extract (CBPE).

c0024

Structural and Dielectric Studies of $Bi_4Ti_3O_{12}$ Plate-like Nanomorphology Prepared By Low Temperature Molten Salt Method

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Polycrystalline ceramic samples of $Bi_4Ti_3O_{12}$ (BIT) have been synthesized at low temperature by adopting molten salt (MSS) route using high purity oxides and NaCl as a flux. The X-ray diffraction studies confirmed the formation of single phase BIT ceramics with orthorhombic crystal structure. The scanning electron micrographs (SEM) revealed the presence of plate-like morphology of the layered structure BIT. The energy dispersive X-ray analysis (EDAX) showed the stoichiometric ratio of the constitute elements present in BIT nanoceramics. The dielectric constant, as well as loss factor, measured at 300K exhibited the dispersion behaviour at low frequencies. The observed high value of dielectric constant and low valve

of loss factor at 300K might establish this ceramic as a promising material for capacitor based devices.

c0025

Microstructural and Optical Properties of Electrochemically Etched Silicon Nanowires (SINWs)

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Silicon nanowires (SINWs) are fabricated by electrochemical etching of silicon using metal-assisted route on silver electroplated silicon (Si) wafer at room temperature. Morphology and optical properties of the prepared samples are investigated through field emission scanning electron microscopy (FESEM), UV-visible reflectance spectroscopy, photoluminescence (PL) and Raman studies respectively. FESEM shows alignment of SINWs in the vertical direction with average length of 24 μm. UV-Visible shows considerably low reflectance of SINWs to that of Si wafer. PL shows an intense peak at around 450 nm. Raman studies complements the FESEM results by showing the peak shifting of SINWs to that of Si wafer due to nano Si structure. Optical properties reveal that SINWs could be a better candidate for optoelectronic applications**.**

c0026

Defect-mediated Photoluminescence Properties of Transitional Metal ions-doped ZnO Nanoparticles

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Transition metal (Ni and Co) ions doped ZnO nanoparticles (TM doped ZnO NPs) were synthesized via a soft-chemical approach. The structural, microstructures, and photoluminescence properties of TM doped ZnO NPs were investigated thoroughly by various characterization techniques. The successful doping of metal ions was evident from chemical analysis and electron mapping using inductively coupled plasma-atomic emission spectroscopy (ICP-AES) and scanning electron microscopy-energy dispersive X-ray spectroscopy (SEM-EDS), respectively. X-ray diffraction and transmission electron microscopy analyses of doped ZnO NPs showed the formation of single-phase wurtzite structure without any impurities. X-ray photoelectron spectroscopy further confirmed the doping of metal ions into the ZnO matrix. The photoluminescence study showed that doped ZnO NPs exhibited the defect-dependent photoluminescence behavior.

c0027

Structural and Electrical Properties of $Ba_{0.9}Sr_{0.1}Ti_{0.9}Mn_{0.1}O_3$

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Nanocrystalline sample of $Ba_{0.9}Sr_{0.1}Ti_{0.9}Mn_{0.1}O_3$ has been synthesized using solid state reaction route. Raman spectroscopy indicates that the sample exists in tetragonal phase at room temperature. The Raman modes shift towards the higher wavenumber indicating the presence of compressive strain with blue shift. Impedance analysis highlights the non-Debye behaviour of the sample. The imaginary part ($-Z''(\omega)$) for the material exhibits a sharp

decrease with frequency indicating the absence of relaxation at room temperature. The a.c. conductivity follows the Jonscher law.

c0029

Heterostructures of Layered Carbon Nanocomposites and Engineered Split-Ring Resonator Array Structures for Wide-band Electromagnetic Shielding

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Micro-assembled, engineered thin film structures of silver arrays have been used along with different carbon Nano composite thin films on flexible substrates for shielding the X-Band (8.2 GHz to 12.4 GHz) Radar range of the electromagnetic spectrum. In this presentation, we discuss on synthesis of flexible thin films of silver arrays of split ring resonators, with varied unit cell dimensions, which are deposited using standard micro-printing technology. These layers are stacked with nanocomposite films of multiwall carbon nanotubes (MWCNTs) in polyvinyl dimethyl fluoride matrix to obtain wide band electromagnetic shielding. Nanocomposites were synthesized using standard chemical methods and thin films were synthesized using dip-coating method. The sandwiched (2 layers of nanocomposites and one layer of resonator array) was packed using hydraulic press and standard lamination technique to yield a compact flexible film, which can be inserted in the X-Band wave guide for further testing. Vector Network Analyzer was used for further studies of absorption. Shielding in entire X-band with the power loss of 27 dB (99.98 % loss) and a minimum of 21 dB (99.92 % loss) is demonstrated here, for MWCNT. Similar results for other carbon composites are discussed in this presentation. A strong interplay of carbon nanocomposites with the array of L-C-R equivalent resonators of varied resonant frequencies shows concomitant suppression in the incident electromagnetic power; the results supported by simulation (CST Microwave Studio) studies as well. This work opens up a strategy to obtain wide band shielding using a combination of optimized nanomaterial composites, heterostructured with engineered metallic resonators.

c0030

Hydrothermal Synthesis and Photoluminescence Study Of Anhydrous Polyhalite $K_2Ca_2Mg(SO_4)_4$

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Nanoparticles of anhydrous Polyhalite $K_2Ca_2Mg(SO_4)_4$ are synthesized by hydrothermal method. The synthesized sample is characterized by powder X-ray diffraction (XRD) to confirm its triclinic crystal structure and to get average crystallite size of the nanoparticles. The UV-Visible spectroscopy is used to estimate the optical band gap energy. The scanning electron microscopy (SEM) is used to study the surface morphology. The photoluminescence study shows that PL emission intensity is found to be 310, 385 and 560 nm.

c0032

Structural, Dielectric and Magnetoelectric properties of Bi^{3+} doped $NiFe_2O_4$ nanoparticles

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Trivalent Bi-ion doped Nickel ferrite nanoparticles exhibiting room-temperature multiferroic properties have been derived using the sol-gel method. The X-ray diffraction pattern is used to confirm the phase purity and lattice parameter of the synthesized samples. Frequency-dependent dielectric properties and magnetoelectric properties of the samples were analyzed. Excellent multifunctional properties show that, it could be a promising candidate for magnetoelectric sensing, memory devices etc.

c0033

Laser Synthesis of Anionic Cadmium Sulfide Cluster Ions: $Cd_mS_n^-$

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Cadmium sulfide cluster ions, $Cd_mS_n^-$ of different stoichiometry have been generated from $CdS_{(s)}$ target material using pulsed laser ablation/desorption ionization technique. The negative ions generated during the laser-matter interaction processes have been analyzed by Time-of-Flight Mass spectrometry. Analysis of the mass spectral data indicates the formation of 6 different binary cluster ion series *viz*., $(CdS)_n^-$, $Cd_nS_{n+1}^-$, $Cd_nS_{n+2}^-$, $Cd_nS_{n+3}^-$, $Cd_nS_{n+4}^-$, CdS_n^- along with abundant S_n^-.

c0034

Substitutional Modification on the Properties of Sr-doped $BiFeO_3$Ceramics Synthesized by Molten Salt Method

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Sr doped $BiFeO_3$ samples with the stoichiometric ratio of $Bi_{1-x}Sr_xFeO_3$(x=0.0, 0.05, 0.10, 0.15, 0.20, mol%) were prepared by molten salt synthesis route using NaCl as a flux. The X-ray diffraction studies of these samples confirmed the phase formation of perovskite type rhombohedral structure of $BiFeO_3$. Furthermore, it also showed the presence of secondary phase of bismuth iron oxide ($Bi_2Fe_4O_9$) in all Sr doped$BiFeO_3$ samples. The XPS analysis revealed the dominance of Fe^{3+} oxidation state in these ceramic samples. The frequency dependent dielectric constant measurements were performed at 300K for x= 0.05 and 0.20 samples from 1kHz to 1MHz which showed the decrease in the value of dielectric constant with increase in Sr concentration.

c0035

Electrochemical Study of Nanosized $Co_{0.5}Zn_{0.5}Fe_2O_4$ Synthesized by Hydrothermal Method

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Herein, we report the electrochemical study of nanosized $Co_{0.5}Zn_{0.5}Fe_2O_4$ synthesized by hydrothermal method. Structural and microstructural characterization has been carried out by powder x-ray diffraction (PXRD) and transmission electron microscopic techniques. UV−vis diffuse reflectance spectroscopy has been performed to analyze the optical property of the sample. The PXRD study suggests that the sample has crystallized as a single-phase cubic spinel ferrite with $Fd\bar{3}m$ symmetry. The average particle size is ~ 19 nm. The band gap of the sample is 1.75 eV. The sample exhibits maximum specific capacitance of 85.5 F/g at 10 mV/s scan rate. The pseudocapacitive behavior of the sample can be ascertained from the non-rectangular shape of cyclic voltammetry curves. The sample can act as a supercapacitor.

c0036

Control of Ferroelectric Dipole Orientation in Ultra-thin Polymer Film for Enhanced Piezoelectric Response

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Effect of annealing in thin-film poly(vinyledene-trifluoride), P(VDF-TrFE) in terms of molecular chain orientation and localized ferroelectric response was investigated systematically. The grazing incidence reflection absorption spectroscopic results indicates the preferential tendency from face-on to edge-on molecular chain orientation upon selective annealing techniques. Piezoresponse force microscopy measurement validates the superior ferroelectric and piezoelectric response in annealed films with vertical piezoelectric coefficient, d33 ~ 16 pm/V compared to as-spun films of ~ 6 pm/V. Furthermore, the dependency on piezo- and ferro-electric responses depending on different types of annealing techniques are also undertaken.

c0037

Synthesis and Characterization of ZnO and Graphene-ZnO Nanorods for NO2 Sensing

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ZnO and Graphene doped ZnO thin films with nanorod structure were synthesized by effective and low cost reflux method. X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), study the properties of prepared samples. Well defined hexagonal shaped vertically aligned nanorod morphology is observed from SEM micrographs. Z axis oriented structure of ZnO rods are confirmed by XRD pattern, NO_2 sensing mechanism and Comparative study of NO_2 sensing of ZnO and Graphene-ZnO films were studied and various parameters were evaluated.

c0038

Study of Structural and Optical Properties of ZnFe2O4 Nanoparticles Prepared by High Energy Ballmilling

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A fine powder of zinc ferrite (ZnFe2O4) was prepared by high energy ball milling, milled for 10 hours, with the balls to powder ratio 8:1 and molar percentage ratio between ZnO and Fe2O3 as 1:1. Solid state diffusion between the precursor materials starts the Zinc ferrite

formation. The process of mechano-synthesis of ZnFe2O4 at room temperature led to the formation of ZnFe2O4. XRD is used to study the phase formation of zinc ferrite and estimated the average crystallite size by using Scherrer's formula. FTIR data reflected proper occupation on Zinc oxide on octahedral site and FeO on tetrahedral site. Optical properties of the synthesized nanoparticles was studies by analysing UV-Vis spectroscopic data.

c0040

Study of photocatalytic activity of pure and CTAB assisted cadmium oxide nanoparticles

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Pure and CTAB assisted CdO nanoparticles have been synthesized via co-precipitation method. X-Ray Diffraction (XRD) spectra confirm the formation of nanoparticles. Formation of oxygen vacancies or defects can be seen from the photoluminescence spectra. Photocatalytic performance of pure and CTAB assisted CdO in the degradation of Methylene Blue (MB) dye in UV light can be seen from the absorbance spectra.

c0041

Impact of Co doping on Mg-Zn Spinel nano-ferrites

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Co-doped Mg-Zn spinel ferrite nanoparticles were prepared via the facile solution combustion method. The crystal structure, lattice parameter, crystallite volume, and the formation of prepared nanoparticles were investigated via XRD. The microstructure and vibrations of tetrahedral or octahedral sites were carried out by TEM and FTIR spectra. VSM analyses are used to study the magnetic properties of the papered samples which revealed the highly magnetic nature of samples.

c0042

Protonation mediated intercalation of selenium in g-C3N4 for the enhanced sunlight driven photocatalytic degradation

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In this study, protonation mediated intercalation of selenium in graphitic-carbon nitride (g-C3N4) has been demonstrated. The observed changes in the XRD and ATR-IR peaks revealed the successful intercalation and improved exfoliation of g-C3N4 layers. A relative red-shift in the optical absorption and emission is observed for protonated Se/g-C3N4, which also found to effectively degrade the rhodamine B dye molecules under sunlight irradiation. This observed enhancement is attributed to the improved surface properties and rich surface-active sites due to the protonation induced intercalation of selenium in g-C3N4 layers.

c0043

Correlation between absorption features and optical transitions from SWCNT based thin film coatings

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In this work, we report correlation between absorption and optical signatures of one dimensional (1D) single walled carbon nanotubes (SWCNTs) as a manifestation of electronic transitions occurring within the sharp van Hove states of valence band, v2 to conduction band, c2. These sharp transitions arising within the van Hove singularities due to the unique 1d structures of SWCNTs correspond to the energy band E22. We demonstrate unique way of correlating 7 absorption energy features with 8 optical transitions depending on the tube diameter and chirality. This assignment has been carried out based on empirical calculations according to the tight binding model approximation. This finding can have direct impact in tuning the bandgap of SWCNTs of specific diameter and chirality for nanoelectronics and nanophotonic applications.

c0045

Bessel Beam Probed Silver Nanostructures Employed As Plasmonic SERS Substrates For Trace Level Detection Of Real-time Explosive and Dye

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In this work, we report the fabrication of exotic silver (Ag) nanostructures (NS) employing a ultrafast Bessel beam utilizing a picosecond (30 ps, 10 Hz) laser pulses. Subsequently, an improved Surface Enhanced Raman Scattering (SERS) response from the Ag NS were thoroughly explored for trace level detection of an explosive (Picric Acid-500 nM) and one dye (MB-5 nM) molecule.

c0046

3D Visualization of Crystallography Information of Hydrothermally Synthesized 2H-MoS2 Nanocrystalline Material

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In this work, we demonstrate the visualization of atomic arrangement of crystal structures and lattice planes of 2H-phase of MoS2 nanocystalline material prepared via inexpensive hydrothermal method. The phase identification and crystallography information are examined through powder X-ray diffraction technique and VESTA-3D theoretical tool. The associated crystal planes are created and displayed. This work is to be useful in modern structure-property relationships.

c0048

Modified Young's Modulus of Carbon Nanotubes with Vacancies: A Molecular Dynamics Approach

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Sp^2 bonding between the carbon atoms inside carbon nanotubes (CNTs) has imparted them astonishing mechanical properties which can be exploited in building super-strong composite materials. A critical study on the variation of their properties under different conditions is necessary to extract their maximum efficiency as filler materials for preparing composites. In the present work the Young's modulus of an armchair, a chiral and a zigzag single-walled CNT of almost same diameter with a number of vacancies at different positions are computationally analyzed to predict their mechanical behavior.

c0049
Low-Temperature Synthesis of Nanocrystalline Silicon-Oxycarbide Thin Films
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Intrinsic nanocrystalline silicon-oxycarbide (nc-SiO_xC_y:H) thin films are prepared by conventional PECVD at a low temperature zone around 170–180 °C, using ~1.6% (SiH_4 + CO_2 + CH_4) in (H_2 + He) diluent, at moderate rf power ~260 W. Crystallinity, grain size and conductivity, in general, improves at elevated substrate temperature. Films possessing adequate crystallinity ~40 %, with (220) crystallographic orientation, good conductivity ~10^{-3} S cm^{-1} and low activation energy ~140 meV, grown at such low temperature seem appropriate for utilization as the window layers in *p-i-n*/*n-i-p* nc-Si solar cells.

c0050
Structural and Optical Properties of Sm Doped α-MnO_2
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Hydrothermal synthesis of bare and Sm doped α-MnO_2 demonstrates the presence of a pure tetragonal phase with space group I4/m. However, after incorporating Sm, the crystal structure of α-MnO_2 rests tetragonal, but the crystallinity reduces. Doping of Sm also increase the number of oxygen vacancies, as measured by X-ray photoelectron spectroscopy. Bare and Sm doped α-MnO_2 have gap of 1.95 and 1.85 eV respectively, as determined by absorption in the UV region. The bandgap in visible region and increase in oxygen vacancy suggest that it could be used as both, a photocatalyst and an electrode in supercapacitors, respectively.

c0051
Development of Diamond-Like Carbon Films with Prominent Nano-diamond Phase
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Diamond like carbon (DLC) films were grown on inexpensive glass substrates, without its pre-treatment or applying dc bias, at a moderate power ~500 W in MW-PECVD. Using C_2H_2 as the precursor gas and utilizing the CH_3 ions extracted by MW plasma decomposition, we have been able to grow DLC films with significant fraction of nanodiamond phase at substantially low temperature of 300 °C. The existence of diamond peak and t-PA peaks, the

maximum magnitudes of I_{Dia}/I_G (~1.05), and minimum magnitude of I_D/I_G ratio (~1.0) in the Raman spectrum indicate good quality of the nano-diamond phase, identified with its <111> orientation in the optically transparent DLC film.

c0052

Optical Properties of Silicon Nanowires Fabricated by Ag –Assisted Chemical Etching

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Silicon and its different nanostructures are already being used extensively in the field of optics, electronics and photovoltaic. Here we have successfully fabricated silicon nanowires on pre-fabricated pyramidal Si substrate (P-Si) by metal assisted chemical etching (MACE) method and the metal used here is silver (Ag). The synthesized nanowires were investigated by Transmission Electron Microscopy (TEM) and its optical properties by PL Spectroscopy and UV-VIS spectroscopy. The NWs on pyramidal Si (P-Si) substrate shows less reflectance compared to planer Si substrate. The PL enhancement has been recorded for P-SiNWs by a factor of 1.3 in comparison to planar SiNWs. All these properties like high aspect ratio structures, enhancement of optical properties taken all together have a great influence on the photovoltaic applications.

c0053

Magnetic Control of Dielectric Permittivity and Electric Polarization Voltage of Polymer Based Nanocomposite Film

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Magnetodielectric and magnetoelectric materials are technologically demanded due to desirable control of dielectric properties and electric polarization. In this work, NiFe2O4/P(VDF-TrFE) nanocomposite films (40 μm) were synthesized using solution casting technique. The magnetodielectric and magnetoelectric properties of these nanocomposites are presented here. Magneto-dielectric study in DC magnetic field range 0-7000 Oe shows increase in permittivity with magnetic field. In addition, room temperature magnetoelectric study shows maximum coupling voltage of 136.4 mV/Oe-Cm at 1.21 kOe DC magnetic field and both the effect was attributed to the presence of mechanical coupling in magnetostrictive and piezoelectric phase.

c0054

Preferential <220> Crystalline Growth of Boron Doped Nanocrystalline Silicon Thin Films by ICP-CVD

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B-doped nc-Si thin films are successfully grown in inductively coupled plasma (ICP) CVD without using additional H_2 dilution to the SiH_4 plasma, by lowering the substrate temperature from 400 °C to 30 °C. The *p*-nc-Si thin film with dominant <220> crystallographic orientation of the nanocrystallites, providing a significantly wide optical

band gap (>1.88 eV) and high electrical conductivity (> 10^1 S cm^{-1}) appears suitable for the nc-Si heterojunction solar cell fabrication.

c0055

Optimization of Process Parameters to Fabricate Uniform, Bead-free Cobalt Ferrite Fibers Through Electrospinning Technique

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The process parameters to fabricate uniform, bead-free cobalt ferrite fibers through electrospinning technique are optimized. To obtain the best quality, bead-free fibers, various electrospinning process parameters such as polymer solution concentration, tip to collector distance, flow rate, and applied voltage were optimized to be 12 wt%, 14 cm, 05 ml/h and 20 kV, respectively. The as spun fibers were then calcined at various heating rates. SEM, TEM, and AFM were used to examine the fiber morphology. Fibers calcined at 800°C with a heating rate of 2°C/min produced bead-free continuous fibers with a fiber diameter of 200 nm. The XRD pattern confirmed the cubic spinel crystalline structure of cobalt ferrite with a crystallite size of 34 nm.

c0056

Carambola-like NiCoP Nanostructure for Efficient OER Activity

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Inexpensive and highly efficient electrocatalysts from earth abundant transition metals are the demand of the hour for renewable energy production. Here we report the successful synthesis of carambola-like nickel cobalt phosphide (NiCoP) through a two-step hydrothermal process followed by the solid-state reaction and its promising employment as an electrocatalyst for oxygen evolution reaction (OER). The as prepared NiCoP exhibits excellent OER activity in 1.0 M KOH solution by reaching 10 mA cm-2 current density at significantly small overpotential of 288 mV. It also showed a relatively small Tafel slope of 83.26 mV dec-1and high durability. The performance is better than the benchmark RuO2 catalyst and the study opens up new possibilities of electrocatalytic OER activity.

c0058

Morphological Transition of The ZnO Hexagonal Nanowires To Cylindrical Nanowires

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Current research paper represents ZnO nanowires (NW's) synthesis by simple chemical method on the seeded quartz substrate. The ZnO NW's were characterized by field emission electron microscopy (FESEM) and X-ray diffraction (XRD) spectroscopy. Morphological evolution of the ZnO NW's from hexagonal to cylindrical shape with the growth time was observed. The growth mechanisms of the NW's as the growth time proceeds were also discussed in this paper.

c0059

Optical and Sensing Properties of Multi-core Gold@Silica Core-shell Nanoparticles

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Multi-core Au@SiO_2 core-shell nanoparticles were prepared successfully via simple chemical synthesis method. The structure and morphology of the synthesized nanoparticles were studied using Transmission electron microscopy (TEM) and their optical properties by UV-vis spectroscopy. A coupling effect on UV-vis spectra was observed due to multiple cores of Au. The electrocatalytic activity of multi-core Au@SiO_2 core-shell nanoparticles was investigated by using cyclic voltammetry technique and it can detect small changes in concentration of glucose. Our present study highlights the influence of multiple Au cores in Au@SiO_2 core-shell nanoparticles on the optical properties and application in the field of glucose sensing.

c0060
Structural And Absorbance Study Of Sm3+ Doped Ca3(VO4)2 Phosphors.
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In this paper, we report the synthesis of Sm3+ (0, 1, 4, and 5%) doped Ca3(VO4)2 phosphor by the urea-assisted combustion process. All the samples are characterized by X-Ray diffraction (XRD), Ultraviolet-visible (UV-vis) spectroscopy, and Fourier Transform Infrared (FTIR) spectroscopy. The XRD result ascertains the rhombohedral crystal structure of all the samples. Absorption analysis manifests that all samples have near UV absorption at 290 nm. The bandgap analysis reveals a decrease in bandgap after Sm3+ doping in Ca3(VO4)2 phosphor. The FTIR analysis confirms all the infrared modes present in the phosphors. We have explained the effects of Sm3+ doping on the structure and absorption of Ca3(VO4)2 phosphor. Thus, our analysis of Sm3+ doped Ca3(VO4)2 phosphor ascertains that it has potential application in lightning devices.

c0062
Synthesis and characterization of sheet shaped MgO nanostructures using paper as a novel solid support
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In the present work we report a novel synthesis and characterization of MgO sheet shaped nanostructures, using simple paper as a solid support. As-synthesised sample was characterized by Powder X-Ray Diffraction (XRD), Field Emission Scanning Electron Microscopy (FE-SEM) and UV-Visible Spectroscopy (UV-Vis). The XRD results confirmed the formation of cubic phase of MgO. FE-SEM micrographs established the formation of MgO sheets like structures in the agglomerated nanoparticles. UV-Vis spectrum reveals absorption property of the MgO sheets. The optical band gap was calculated to be 3.5 eV, which is less than the bulk MgO value. These results corroborate the formation of MgO sheet shaped nanostructures.

c0063
Magnetic Study of Ni doped CdTe Nanoparticles

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Pure and nickel (Ni) doped cadmium telluride (CdTe) nanoparticles have been synthesized by chemical route. The X-ray diffraction patterns at room temperature show the cubic phase of the samples. The average crystallite size of pure and doped CdTe is found to be ~ 15 nm using Debye-Scherrer formula. The field dependent (M-H) and the temperature dependent (M-T) magnetization of the samples have been considered at room temperature and low temperature (2 K). M-T measurement at 500 Oe has been carried out under zero field cooled (ZFC) and field cooled (FC) conditions. There is a sharp peak in M-T measurement for pure CdTe nanomaterials shows the magnetic transition temperature from diamagnetic to ferromagnetic transition.

c0064
Structural and Optical Properties of Green Synthesized Zirconium Oxide Nanoparticles
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Green synthesis method was adopted to prepare the zirconium oxide nanoparticles. The prepared zirconium oxide nanoparticles were characterized by powder X ray diffraction, Raman Spectroscopy and UV-visible spectroscopy to investigate the structural and optical properties respectively. The powder X- ray diffraction data showed that the green synthesized zirconium oxide nanoparticles belong to cubic structure and the lattice parameter was determined. Raman Spectrum of the green synthesized zirconium oxide nanoparticles confirmed that the prepared samples are cubic crystalline structure. Optical absorbance of the green synthesized zirconium oxide nanoparticle was studied from the diffuse reflectance spectra and it showed that the prepared nanoparticles are opaque in the ultraviolet light region.

c0065
Characterization of TiO_2 and Zn doped TiO_2 Nanofibers for DSSC applications
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We have synthesized one dimensional TiO2 nanofibers using electrospinning technique and Zn2+ ions are doped over the TiO2 nanofibres through a simpler impregnation technique. Both the undoped TiO2 nanofibres and Zn doped TiO2 nanofibers were analyses for their structural and optical properties. The fabricated TiO2 and Zn doped TiO2 photoanodes are used in DSSC and its photo conversion efficiency (PCE) was found to be 3.47 and 2.51%

c0066
Structural And Optical Studies Of Dy3+ Doped ZnMoO4 Phosphors.
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In this work, un-doped and Dy3+ doped ZnMoO4 phosphors have been prepared via a facile auto-combustion method. The diffraction peaks of the XRD pattern confirm the triclinic phase of doped and un-doped ZnMoO4. Optical studies have been investigated via UV-Vis analysis and photoluminescence analysis. UV-Vis absorbance spectra of ZnMoO4 and Dy3+ doped ZnMoO4 confirm the shift in bandgap with Dy3+ doping. Photoluminescence excitation spectra represent a broad excitation band centred at 302 nm for host phosphor, corresponds to [MoO4]-2 band. Photoluminescence emission spectra represent broad emission spectra centred at 518 nm corresponds to [MoO4]-2 energy band. Some intense peaks are observed at 495nm, 575 nm, and 661 nm, corresponds to 4F9/2→6H15/2, 4F9/2→6H13/2, and 4F9/2→6H11/2 transitions of Dy3+ ion under the host's excitation at 302 nm. The chromaticity coordinate (CIE) of the Dy3+ doped phosphor represents the overall emission in the yellowish-white color which suggests that Dy3+ doped ZnMoO4 phosphors can be a better candidate to realized in white light-emitting diode (w-LED).

c0067
Study of Structural and Optical Properties of Europium Ion Activated Bismuth Oxide Nanophosphors
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This paper presents a study of structural and optical properties of un-doped and a series of Eu3+ ion doped bismuth oxide nanophosphors synthesized via a facile, low-cost and room temperature co-precipitation method. X-ray diffraction (XRD) analysis confirms the monoclinic crystal structure of the samples without any trace of impurity. Optical properties of the samples have been investigated using UV-Vis and photoluminescence (PL) spectroscopy. A slight increment in the band gap has been observed in the doped samples (2.79-2.81eV) as compared to the bismuth oxide host (2.77eV). The emission intensity has been augmented sufficiently in 7 mol% Eu3+ doped Bi2O3 nanophosphor. Thus, our study corroborates an evident red-shift in the aforementioned optimized composition and suggests that it is a potential candidate for lightning and display devices.

c0068
Interband Transition in Plasmonic Nanomaterials and its Application for UV Light Harvesting
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In this study, we have shown the applicability of interband transition generated charge carriers in plasmonic nanosystem for the fabrication of highly responsive and ultrafast UV photodetectors. Two different devices are fabricated – one with gold nanoparticles (Au NPs) and the other with titanium nitride (TiN) nanoparticles. In both the devices, plasmonic interband transition generated photocurrent is coupled with the excitonic-pyroelectric current of non-centrosymmetric wurtzite zinc oxide (ZnO) and as a result, the performance of the devices enhances significantly. Both the devices show very promising performance in self-powered mode. However, the Au NPs based device shows very high performce in the photoconductive mode also.

c0069

Ultraviolet Emission from Gd^{3+} Doped $NaSrBO_3$ Orthoborate for Medical Applications

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Gd3+ doped sodium strontium borate phosphors were prepared at different concentrations of Gd^{3+} ions and examined for their luminescence properties. The material was synthesized by solid-state reaction using carbonates as initial materials. Powder X-ray diffraction (PXRD), Scanning Electron Microscopy (SEM) and photoluminescence studies were done to examine the structural, morphological and luminescence properties of the material. The PXRD results reveal that the $NaSrBO_3$ has a monoclinic phase with the space group. The luminescence spectra of the material show UV emission at 312 nm at different excitation wavelengths assigning to the Gd^{3+} emission.

c0070

Exploration of Polythiophene (PTh) Thin Films for Chemiresistive Gas Sensors

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In the present investigation, the effect of the oxidant concentration of PTh thin films on gas sensing performance was studied and discussed. The deposited thin films were characterized for their structural, morphological, optical, compositional, and electrical properties. The increase in oxidant concentration leads to increased film porosity and thickness (94nm to 294nm) due to systematic development of organised polymeric structures (from agglomerated structure to nanobelts). The amorphous structure of PTh was confirmed by using the X Ray Diffraction technique. The surface morphology was observed in Scanning Electron Microscopy images specified the formation of nanobelts. The gas sensing measurement study indicated that the PTh thin film sensor is highly selective and sensitive to NO2 gas. The maximum gas sensitivity of 55% for the PTh thin film sensor is observed for 1:2.5 monomer to oxidant ratio. The PTh thin film based sensor shows an excellent response to NO2 gas at even low gas concentrations (10 ppm) along with flexibility, low cost, portable and wearable nature. The sensor exhibits not only high sensitivity but also good selectivity towards NO2 gas.

c0072

Using metal ion embedded nanocomposite glass materials - For biosensing application.

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The physicochemical properties of metal embedded nano clusters are totally different from those of the bulk materials. The nanocomposite nanocluster depends on their size, shape and the chemical composition and they have more reactivity which is taken considerably larger

than those of the bulk by orders of magnitude with size. Optical absorption spectroscopic analysis was done on the metal nanocluster composite glasses, and the spectra are well studied as a function of various post ion-exchange treatments and different sizes. The noble metal nanoclusters play an important role for nanobiomedical and modern optical devices. Raman scattering is a nondestructive tool for probing the composition and symmetry of nanocrystalline semiconductors and insulators. The present paper explored the single and bi-metallic nanoclusters embedded in soda–lime glass that is prepared by ion-exchange method. The ion-exchanged glasses are annealed by different methods. These samples exhibit surface plasmon and surface enhancement effect. As size effects are an essential aspect of nanomaterials, the effect of size on the optical absorption metal nanoclusters shall be studied through optical absorption, SERS. From this study, we find optimized SERS substrate for single and different molecule detection

c0073

Antioxidant and cytotoxic potential of Diosgenin nanoparticles against Ehrlich ascites carcinoma (EAC) cells

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Diosgenin (DG), a naturally occurring steroidal saponin from therapeutic herbs, is reported to be a potential natural antioxidant and anticancer agent. However, its clinical application was limited due to its high hydrophobicity and poor bioavailability. We developed a nanoparticle platform to increase its clinical efficiency by producing PLGA-DG nano-particles and have been characterized by DLS, FTIR and FE-SEM. We evaluated the cytotoxic and antioxidant activity of PLGA-DG NPs against Ehrlich Ascites Carcinoma (EAC) cells and in EAC- bearing mice. PLGA-DG NPs has shown potent cytotoxicity against EAC cells. Very significant antioxidant effects were seen in liver superoxide dismutase (SOD) and catalase (CAT) activity and in malondialdehyde (MDA) content of EAC- bearing mice compared to DG. These findings revealed the cytotoxic and antioxidant potential of PLGA-DG NPs which was significantly increased by the above said nano-formulation.

c0074

Green exfoliation-assisted evolution of g-C3N4 rods and their structure-modification induced photocatalytic activities

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One dimensional rod-like structures of g-C3N4 (GCN) have been synthesized via the ultrasonic-assisted green treatment process using Azadirachta indica A. Juss (neem) extract as exfoliating-cum-shape directing agent. It is observed from various studies that the green-modified GCN is rich in amine groups that effectively bridge the heptazine and triazine networks, which eventually gives rise to the structural, morphological, optical and photocatalytic properties of GCN as compared to the conventional-GCN.

c0075

Stractural, Optical and Electrical Properties of $Cu_{1-x}Fe_xO$

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Semiconducting CuO has interesting electrical and electronic properties which can be tuned by Fe doping. Crystalizing in a monoclinic structure with (C2/c) symmetry sol-gel prepared CuO nanoparticles were synthesized. A comparison of the structural properties along with the changes in optical as well as the electrical properties are reported for these two samples. The electrical conductivity degrades with Fe doping while band gap decreases.

c0076
Flow Synthesis of Ultra Small Gold Nanoparticles in PTFE Microchannel
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Flow synthesis of ultrafine colloidal gold nanoparticles (AuNP) below 5 nm in a microreactor is reported. The micro reactor is essentially a 0.8 mm diameter PTFE micro capillary coiled helically. The gold precursor (tetrachloroauric acid) along with trisodiumcitrate are premixed and infused into the microbore tube kept immersed inside a hot oil bath using a syringe pump. Trisodiumcitrate acts as the reducing as well as stabilizing agent. The synthesized AuNP are less than 5 nm in size and are mostly spherical in shape. Systematic studies are conducted to investigate effect of residence time on particle size. Larger sized particles are seen to form at shorter residence time. A higher trisodiumcitrate to gold precursor ratio is seen to favor formation of smaller nanoparticles. A mechanistic picture of the synthesis process is proposed to justify the experimental trends.

c0077
Protein Coated Nanoparticles: Biodistribution Study in Dalton Ascites Lymphoma Bearing Mice
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The field of bio-nanotechnology has opened up new avenues for various aspects. This study reports the synthesis, characterization and pharmacological properties of albumin coated biogenic silver nano-formulated chlorogenic acid (AgNPs-CGA-BSA). AgNPs-CGA-BSA was characterized by DLS, XRD and SEM. AgNPs-CGA was crystalline with a uniform distribution in shape and size. AgNPs-CGA-BSA was mostly crystalline with a uniform spherical shape. It may be considered as a stable new nano-drug against cancer in future.

c0078
Role of Solvents on Exfoliation and Optical Properties of Hexagonal Boron Nitride
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2D materials like hexagonal boron nitride nanosheets (hBNNS) are remarkable nanostructured material that find a lot of technological applications thus demanding easier and faster ways for its synthesis. In this work, liquid phase exfoliation method is followed for the synthesis of a few-layers hBN. For this purpose, three different solvents were used. A suitable solvent activates the exfoliation of bulk hBN to mono or a few layered hBNNS and at the same time it offers stability of the suspension. UV-Vis spectroscopy was employed to

quantify the optical band gap of synthesized hBNNS. Raman spectroscopic results were used for estimation of approximate number of layers. The Raman results support the UV-Vis findings. This study will help in selection of suitable chemical solvents for synthesis of hBNNS with higher yield and stability.

c0080

Mesoporous ZnS/NiS Nano-Composite for Multi-Functional Visible-Light-Driven Applications

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Present study reports the facile synthesis of phase separated ZnS/NiS nanocomposite by two-step solvothermal approach. Structural analysis showed the formation of highly crystalline uniform-sized, sharp-edged hexagonal pyramidal particles. Transient photocurrent response and electrochemical impedance spectroscopy showed enhancement in the electron-hole separation and their mobility, which ultimately resulted in decreased charge-transfer distance, improved electrical conductivity and reduced charge-transfer resistance. Moreover, the synthesized nanocomposite also showed a significant improvement in the catalytic behavior which was attributed to the restructuring of surface properties and modification in the band structure of the constituent phases.

c0081

The Effect Of Temperature Variation On Structural Property Of NiFe2O4/ZnO Nanocomposite

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Nanocomposites NiFe2O4/ZnO were synthesized by two-step methodology at different annealing temperatures (400◦C, 500◦C and 700◦C). Zinc oxide (ZnO) nanoparticles having unique physical and chemical properties synthesized by co-precipitation method. X-ray diffraction (XRD) is used to confirm the formation of both NiFe2O4 (NFO) and ZnO phases in NiFe2O4/ZnO nanocomposites. FTIR is used to determine the functional groups present in the prepared sample in the range of 400-4000 cm^{-1}. Crystallite size was calculated using Debye Scherrer formula and are found to be 36.28 nm, 36.27 nm for NFO and ZnO respectively.

c0085

Annealing Effects on 100 keV Silicon Negative Ions Implanted SiO_2 Thin Films

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SiO_2 thin film of thickness 300 nm grown on p-type silicon substrate was implanted with 100 keV silicon negative ions for the fluences of 1 x 10^{16}, 5 x 10^{16} and 1 x 10^{17} ions cm^{-2}. The implanted samples were annealed at the temperature of 900 °C. Ultraviolet visible near-infrared spectroscopy technique has been used to investigate the implanted SiO_2 thin film samples before and after thermal annealing. Thermally annealed samples showed higher transmittance as compared to non-annealed samples. This may be attributed to the creation

of new SiO_x phase in the SiO_2 matrix at higher temperature. The energy band gap value was found to increase after thermal annealing. This effect may be related to the formation of silicon nanoclusters.

c0086

Fe_3O_4 loaded g-C_3N_4 layered composites for photoreduction-driven degradation of organic dye molecules under sunlight

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Magnetite (Fe_3O_4) particles loaded g-C_3N_4 (GCN) layered composites have been synthesized via melamine condensation-cum- precipitation method. The characteristic presence of Fe_3O_4 in g-C_3N_4 is confirmed from the XRD patterns and a reduced bandgap energy of 2.38 eV is observed for Fe_3O_4/GCN composite, while it is 2.51 eV for bare-GCN. It is proposed based on the relative band edge potential of Fe_3O_4 and GCN that the photocatalytic process could have largely driven by reduction-mediated degradation process rather than oxidation-mediated process towards degradation of rhodamine B under sunlight irradiation.

c0087

Quantifying Pattern Formation During Evaporative Assembly of Colloids in a Drying Droplet on Porous Substrate

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Evaporative-drying of a colloidal droplet leads to the formation of various patterns on a porous substrate. Such pattern formations on porous membranes have been investigated using scanning SAXS to understand the structural correlation of the self-assembly process of colloidal nanoparticles. Parameter space diagram, revealing the relationship between three competitive processes of flow, evaporation, and coagulation, which determines the colloidal assembly, have been generated by feasible computation model corroborating the experimental SAXS data. The phase diagram demarcates different domains of evaporative assembly processes on porous substrate leading to various forms of dried patterns of correlated nanoparticles.

c0088

Structural Investigation of $NdFeO_3$-$PbTiO_3$ Solid Solution by Rietveld Refinement and Raman Spectroscopy

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The preparation of $NdFeO_3$-$PbTiO_3$ nano composite was carried out by mixing of both the samples in proposed proportions. The presence of tetragonal phase of $PbTiO_3$ in the orthorhombic crystal structure of $NdFeO_3$ is established by Rietveld refinement of XRD data. W-H plot confirms the nanocrystalline behaviour of the sample. The room temperature Raman analysis of the composite sample indicates the presence of *Pbnm* and *P4mm* symmetry in the system and show blueshift in the spectra.

c0090

Structural Properties of Sm and Co co-doped BiFeO3

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The 5% Sm & Co co-doped $BiFeO_3$ sample are processed by solid state reaction route ,in order to study structural properties of the sample, The Reitveld Refinement has been performed using rhombohedral (R3c) symmetry. The change in lattice parameter confirms the substituion of Sm at Bi. site and Co at Fe site respectively. The particle size using debye scherrer equation and W-H plot confirms the nanometer scale particle size. Secondary phase of $Bi_2Fe_4O_9$ and sillenite is also confirmed.

c0093

Evaluation of Ni Doped SnO_2 Nanocomposites for Selective Cadmium Detection in Wastewater

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An electrochemical sensor based on Ni/SnO_2 nanocomposites prepared by co-precipitation method has been reported for the detection of Cd^{2+}. Cyclic voltammetry (CV) studies indicated that the developed sensor has superior selectivity towards Cd^{2+} in comparison to its response towards other toxic metal ions. The sensor could detect Cd^{2+} in a wider linear range from 1 to 200 ppb with a detection limit of 0.4 ppb. These superior sensor responses are attributed to the synergetic effect of nickel doping and SnO_2. In particular, the enhancement of the charge transfer ability of the synthesized nanocomposites leads to an improved response characteristic.

c0094

Synthesis and Characterization of Cost-Effective Calcium Titanate Nanostructured Powder and Fibers for Display Applications

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Calcium titanate ($CaTiO_3$) nanostructured powder has been synthesized by modified sol-gel method using eggshell (ES) as the precursors for CaO and titanium (IV) isopropoxide as a source of titanium oxide. The powder X-ray diffraction peaks demonstrate pure phasic structure of calcinated sample as orthorhombic. The average crystallite sizes were calculated by Debye scherrer's formula and are in the range of 25–30 nm. FTIR results confirmed the characteristic functional groups of $CaTiO_3$. Furthermore, calcium titanate nanofibers with controlled microstructure were fabricated by electrospinning method. Finally, from the present study it can be concluded that the presented sol-gel synthesis could be novel way for producing nano $CaTiO_3$.This new nanostructured material and nanofibers could be low-cost potential candidates for the display and lighting applications.

c0095

Synthesis and Photocatalysis of ZnO Nano/Micropeony

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Large scale, low temperature and template free synthesis of hierarchical ZnO nano/micropeony using simple hydrothermal method. The morphological, structural and optical properties of the as-synthesized ZnO products were studied using various physico-chemical characterizations. The ZnO morphologies reveal well defined and self-assembled interconnected sheet-like structures and which is observed to be sensitive to the hydrothermal temperature. The possible growth mechanism is discussed briefly. Furthermore, the photocatalytic activities of ZnO nanostructures toward methylene blue dye under ultraviolet light showed enhanced activity over commercial Degussa P25. Larger surface area, high adsorption rate, large charge separation and the slow recombination of electrons/holes in ZnO establish nano/micropeony as favourable morphology for good photocatalysis. Being wide band gap semiconductors, these unique nanostructures will have prospective application in ZnO based dye sensitized solar cells.

c0096

Low temperature synthesis and optical properties of ZnO nanoparticles

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ZnO nanoparticles were synthesized through the thermal decomposition method and were characterized by using X-ray diffraction (XRD) and UV-Visible (UV-Vis.) spectroscopy. XRD study confirmed the synthesis of ZnO nanoparticles at 250 ℃ with a crystallite size of 19.4 nm. UV-Vis. spectra showed a characteristic peak at 362 nm. Energy bandgap was calculated using the numerical derivative method and the Tauc plot method. The concentration of ZnO nanoparticles was also computed using Beer-Lambert law.

c0097

Zirconium incorporated 1-D titanate nanostructures and its application in defluoridation of water

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In this work, the authors present an efficient method of inclusion of Zr(IV) ions in the interlayer region of 1D titanate nanostructures, resulting in the formation of zirconium intercalated titanate nanostructure (ZTNS). The phase, tubular morphology and elemental analysis of the material was confirmed by XRD, TEM and EDS respectively. The developed material proved to be a promising adsorbent for defluoridation of water. Fluoride contamination of water is a problem that is affecting people worldwide. There is an emerging need for efficient defluoridating adsorbents. The successful inclusion of the Zr into the titanate nanostructure leads to enhanced fluoride adsorption, with 95% fluoride adsorption efficiency. The high defluoridation capacity of the material was obtained using low adsorbent dosage and short contact time period.

c0098

Cobalt Doped Hydroxyapatite as Efficient Adsorbent for the Removal Congo Red Dye

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Removal of carcinogenic industrial effluents is a great challenge in water treatment. In this work we synthesized nano structured Hydroxyapatite (HAp) and Cobalt (Co) Doped Hydroxyapatite via facile wet chemical precipitation technique. The dye removal efficiency and adsorbent - adsorbate interaction kinetic study were conducted against the aqueous solution of Congo Red (CR) dye. The reduced crystallite size (0.49 nm for 10CH) and high surface area ~ 193.97 m2/g is responsible for the high dye removal efficiency (84.78%). The pseudo second order kinetic reaction shows better fit for this mechanism in which electrostatic interaction and chemisorption process are involved. HAp and Co-HAp could be used as a potential adsorbent for the removal of dye molecules from contaminated water.

c0099

Surface Potential Alternation of Graphene Using hBN Substrate

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Hexagonal boron nitride (hBN) as a substrate relaxes graphene surface; the conventional SiO_2 imposes microstrain on pristine graphene whereas a little lattice mismatch with graphene makes hBN a perfect substrate of graphene. Raman spectroscopic studies show the relaxation in the lattice structure of graphene. AFM image-derived surface roughness shows a decrease in surface roughness of graphene when hBN is used as a substrate in the place of SiO_2. The work function enhancement as mapped from scanning Kelvin probe microscopy supports the morphology of graphene where surface roughness and work function are inversely proportional.

c0100

Synthesis of Boron Carbon Nitride (BCN) by Thermal Annealing of hBN in Graphitic Environment

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A novel synthesis method of boron carbon nitride is presented here. For this purpose, thin film of hBN on SiO_2/Si was annealed at ~1000°C in presence of graphite powder. The whole process was performed in a vacuum-sealed quartz tube. Confirmation of presence of carbon atom in synthesized BCN was ascertained by Raman spectroscopy. Carbon bonding with boron and nitrogen atoms was confirmed by FTIR spectroscopy. This work has opened up a sustainable, fast and reliable method of synthesizing boron carbon nitride which finds excellent applications in optoelectronic devices.

c0102

Facile Synthesis and Characterization of ZnO/NiO Composites for Antibacterial Applications

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Semiconducting oxide based nanocomposites have gained more attention in environmental applications. Present investigation is devoted to prepare ZnO/NiO nanocomposites (1:1 ratio) using a facile co-precipitation method. XRD patterns exhibited diffraction peaks corresponding to hexagonal wurtzite structure of ZnO and face centered cubic structure of NiO. UV-vis spectrum shows the optical property of the prepared samples. Band gap energy of ZnO/NiO samples is 2.93 eV. HRTEM image shows the shape and structure of ZnO/NiO composites that containing randomly oriented spherical and pebble shaped particles. From antibacterial study, ZnO/NiO composites show a good antibacterial activity against E. coli bacteria.

c0103

Possible Origin of Local Symmetry Breaking in Transition Metal Doped SnO_2 Nanocrystals

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Three prototype systems of transition metal doped SnO_2 nanocrystals – $Sn_{1-x}Co_xO_2$ (x = 0.00, 0.02, 0.03 and 0.04), $Sn_{0.97-y}Co_{0.03}Ni_yO_2$ (y = 0.02 and 0.04) and $Sn_{1-z}Mn_zO_2$ (z = 0.02 and 0.04), with an average crystallite size in the range of ≈ 11 nm to ≈ 6 nm, have been studied. A study of the lattice dynamics of the nanocrystals indicates that there exists a local inversion centre symmetry breaking on Co and Mn doping in the nanocrystals whereas the symmetry gets partially restored on codoping with Ni (*i.e.*, in $Sn_{0.97-y}Co_{0.03}Ni_yO_2$), although all the nanocrystals retain the long range tetragonal SnO_2 phase throughout the doping concentration. An analysis of the electronic structure of the host in these nanocrystals reveal a change in relative concentration of an Sn-related point defect, $Sn_i^{\cdots}$ *w.r.t.* the host Sn_{Sn}^{x}, in synchronicity with the local modulation of inversion symmetry, indicating this point defect to be a possible origin of the observed local symmetry breaking in transition metal doped SnO_2 nanocrystals.

c0104

Synthesis and Characterization of Yttrium doped Carbon Nitride

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Undoped and yttrium-doped Carbon nitride (Y/ C_3N_4) was synthesized by using melamine as a precursor and yttrium as a dopant material. The prepared samples were characterized by X-ray diffraction pattern, UV-Vis absorption and FTIR analysis. The results confirm the formation of Y-doped C_3N_4. Introduction of Y species effectively extends the spectral response of C_3N_4 from ultra-violet to visible region and it does not modify the crystalline

structure of C_3N_4. The results suggest that Y-doped C_3N_4 may use as photo catalytic material because of its enhanced absorption property.

c0106

Uncapped SnO2 QDs for Efficient Photocatalytic Degradation of Dye

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SnO2 nanoparticles in size less than the Bohr exciton radius (QDs) were synthesized by a simple chemical method without capping agent. It is characterized by various techniques such as XRD,UV–Vis, Photoluminiscence (PL) and BET. The photocatalytic degradation of Methylene blue (MB) dye was investigated by synthesized SnO2 and commercial TiO2. Only complete degradation of MB is achieved by SnO2 within 16 min with a rate constant of 0.13 min-1.Such exceptional catalytic performance compared to TiO2 is attributed to the crucial role of high defects density that delays the recombination process.

c0107

Structural and Thermal Properties of Bare Polypyrrole (PPy) and TiO2/PPy Composite

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Current research article emphasize on structural and thermal properties of the polypyrrole and it's composite with TiO2. The composites were characterized using FTIR and TGA. FTIR revealed the presence of TiO2 in polypyrrole matrix. The shift in N-H peak may be attributed by TiO2 doping in the polypyrrole. The interactions between TiO2 and polypyrrole enhanced its thermal stability as confirmed by TGA analysis of PPy and TiO2/PPy composite.

c0108

Structural and Optical properties of $M_{0.01}Ni_{0.99}O$ (M = Li, Na and K)

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$M_{0.01}Ni_{0.99}O$ (M = Li, Na and K) samples were synthesized via sol-gel process. X-ray diffraction (XRD) spectrum of synthesized material confirmed the formation of metal oxide nanoparticles. WH-UDM (Williamson Hall Plot Uniform Deformation Model) has been used to calculate the crystallite size of the synthesized materials. The optical properties of Lithium, Sodium and potassium doped Nickel Oxide, have been done using UV-Vis and Photoluminescence (PL) study.

c0110

Enhancement in Field Emission behavior of RGO emitter in N2 ambience under high vacuum conditions

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A facile approach to synthesize Reduced graphene oxide (RGO) nanosheets in large scale through thermal evaporation of exfoliated graphite oxide precursor is reported. We have investigated the gas dependent field emission (FE) behavior of the RGO emitter under ultra high vacuum (UHV, ~1x10-8 mbar), and N2 base pressure of ~1x10-6 mbar. Interestingly, the RGO emitter exhibits relatively lower values of turn-on and threshold fields in N2 ambience. The observed enhanced electron emission behavior in N2 ambience is attributed to modulation of the work function of RGO emitter.

c0111

The Electronic properties of Germanene nanoribbon doped with boron and nitrogen : Ab initio study

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Germanene nanoribbons (GeNRs) possess electronic properties similar to carbon based materials like graphene. The effective boron and nitrogen substitutional doping at edge and centre site alters electronic properties of zigzag germanene nanoribbons (ZGeNRs). The study conducted using spin unpolarized density functional theory (DFT) calculations. We have calculated the total energy, fermi energy and band gap. The substitutional boron and nitrogen atoms changes property of material from semi-metal to metallic in ZGeNR. These materials have potential application in spintronic devices.

c0112

Synthesis and Characterization of Monodispersed Polystyrene Spheres and Hydrophilic Sulfonated Polystyrene spheres.

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The synthesis of monodispersed polystyrene spheres has got plenty of attention nowadays. Controlling the particle size is the most crucial task in the synthesis route. This study aims to synthesize monodispersed cationic polystyrene spheres using the single-step facile method. We could control the size of the particles by varying the amount of monomer used. We found that the amount of monomer got proportional dependence on the size of spheres. It was found that the synthesized PS spheres to be highly hydrophobic. This hydrophobicity may be a limitation in many cases when sensing applications come into play. We can overcome this limitation by modifying the polystyrene spheres by a method called sulfonation reaction. After sulfonation, polystyrene spheres are hydrophilic and can be used as templates for sensing applications.

c0113

Influence of Ni doping on the structural and ferroelectric properties of BaTiO3 solid solution

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In the present study, we have synthesized undoped and Nickel doped BaTiO3 ceramics with their compositional formula BaTi1-xNixO3 (x=0 and 0.08) using sol-gel auto combustion process. X-ray diffraction technique were used for the phase purity confirmation. Rietveld refinement analysis ensures that undoped sample are in tetragonal phase within P4mm space group while doped sample have both tetragonal and hexagonal phase within P4mm and P63/mmc space group. It means that the transformation of phase from tetragonal to hexagonal is strongly depend upon the Nickel doping. The average crystallite found to be in the range of 37-51 nm using Scherrer's equation. Various unit cell parameters were determined through Rietveld refinement studies. Ferroelectric measurements demonstrate that the pristine sample has maximum values of remnant polarization (Pr) and maximum polarization (Pm) which decrease linearly with the increase in Ni doping suggesting doped samples suggesting system is going towards centrosymmetric phase.

c0114

Unraveling the Enriched Photoluminescent Tunability in Heteroatom Doped Cdots Derived from Folic Acid

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Carbon dots with tunable photoluminescence are promising candidates for biosensing and bioimaging applications which require long wavelength region of visible spectrum1. Since bare cdots exhibit blue fluorescence with low quantum yield, functionalization (heteroatom doping and surface modification) is inevitable for obtaining unique fluorescence properties. Functional groups having Nitrogen and Fluorine can increase the delocalization of electrons and induces more Π conjugation leading to redshifts in its fluorescence2. Broad emission spectrum of Cdots is indispensable in detection applications, since the entire spectrum of Cdots can be detected. We synthesized N, F- heteroatom doped Cdots derived from folic acid through a simple hydrothermal treatment. They exhibited a broad emission spectrum with a FWHM of ~ 70 nm. FTIR spectrum confirms the presence of oxygen functional groups in the as synthesized CDs. NH4F, and NH4OH doped Cdots produce longer wavelength emission (green emission) on higher wavelength excitation due to the delocalization of electrons. The NH4OH doped Cdots (NFCNDs) exhibited a redshifted broad emission from bare Cdots under a 380 nm excitation. Considering the fluorescence origin, it was understood that the blue emission is from single emission center and the multi-exponential decay fitting further confirms the presence of several emission states within a single center3. The broad emission spectra of NFCNDs demonstrate the great potential of Cdots in detection sensitivity.

c0115

Tuning Specific Absorption Rate Of Fe_3O_4 By Forming An Inverted Core/shell NiO@ Fe_3O_4 For Effective Magnetic Hyperthermia.

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One of the leading causes of death in today's world is cancer and it has become a major problem worldwide. Hyperthermia is one of the emerging cancer therapies that can effectively kill the tumour cells. In this work, we have tuned the magnetic properties of Fe_3O_4 (F) magnetic nanoparticles (MNPs) to enhance the heating efficiency through magnetically

exchange coupling at the interface of the two materials by forming an inverted core@shell (CS) nanostructure NiO@ Fe_3O_4 (Ni@F) and we have reported higher specific absorption rate (SAR) for the CS over the single material F attributing to the interface exchange coupling. The formation of CS nanostructure is confirmed through TEM image and the magnetic study reveals an exchange bias effect (EBE) phenomenon which is an evident of strong magnetically exchange coupling at the interface of the CS nanostructure.

c0117

Photocatalytic performance of visible light irradiated Tin disulfide (SnS2) nanoparticles prepared with different aged times

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It is proposed to enhance the photocatalytic performance of Tin disulfide nanoparticles by changing the aging time for the preparation of the samples. The effect of aging time on the structural, optical, and photo catalytic properties of the SnS2 nanoparticles were investigated. The powder X-ray diffraction analysis study reveals that the prepared samples belong to the hexagonal crystal system and displays that with the increased synthesis time, the crystallinity of the prepared samples have been improved greatly. Likewise, the UV-Visible study reports that with the increased aging time, the absorption edge of SnS2 nanoparticles has been extended to visible region with the absorption cut off around ~570nm (band gap 2.17eV). The extension in the absorption edge promotes the photo catalytic performance of the SnS2 nanoparticles significantly with the utilization of less energy for electronic transitions. Thus, the SnS2 samples obtained with different aging periods demonstrate the nanospheres with bigger crystallite size, narrower bandgap and enhanced catalytic efficiency and these qualities make them as an efficient material for environmental air and water filtration and purifications.

c0118

Rough Bimetallic Substrate for Surface -Enhanced Raman Spectroscopy Application

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For analytical application in the field of sensors to be used in the point of need, low-cost Surface-enhanced Raman spectroscopy (SERS) substrate using rough copper as a base, are an alternative. Bimetallic nanostructures are getting more attention due to high sensitivity, high density of hot spots and high enhancement factor. Our novel approach is based on the deposition of silver nanorods (AgNRs) on rough copper that allowed for the determination of trace levels of Rhodamine 6 g with a limit of detection of 10-4M. These results show the promise of a solid substrate decorated with AgNRs for SERS application.

c0119

Optical And Structural Properties of Tb:CePO4 Nanowires

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Pure and 5 wt% Tb doped CePO4 nanomaterials (nanowires) were synthesized using chemical route and were characterized for their optical and structural properties. Thesenanomaterials wereprepared using of Ce and Tb nitrates as starting materials. FromFTIR data, it was confirmed that pure CePO4 has formed without any FTIR sensitive chemical impurity and contains the desired PO43− tetrahedrons which are characteristics of the phosphate group.UV-Visible spectrum also shows characteristic peaks from monoclinic CePO4 structure and corresponding absorption versus energy plot provided the values of bandgaps to be ~3.6 eV (pure) and ~3.9 eV (doped) confirming the modifications upon doping.The experimental work presented here would be helpful in understanding the photoluminescence behaviour and its dependence on doping amount in future.

c0121

Fabrication of high-resistivity silicon nanowires for infrared sensing application

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This paper presents fabrication of high-resistivity (ρ> 1000 Ω-cm) silicon nanowires (SiNWs) for infrared sensing application. The SiNWs structures are fabricated by using cost effective Metal Assisted Chemical Etching (MACE) process. After the synthesis the morphological, structural and reflectance of SiNWs were analyzed by using SEM, XRD and FTIR respectively. The fabricated SiNWs having length ~7.8-20 □m with diameter tens of nanometer, found to be (111) oriented. The FTIR study of the SiNWs showed drastically decreased transmittance (<1%) and reflectance (0.1-6%) characteristics in comparison to the bare Si (transmittance: 20-30%; reflectance: 35-40%). It infers an excellent IR absorption material for futuristic infrared sensing applications. The reduced transmittance and reflectance characteristics are appearing due to the plasmonic effect of the SiNWs.

c0122

Morphological, Optical and Electrical analysis of ZnO nanorods grown by hydrothermal method for vibration sensor application

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Zinc Oxide (ZnO) nanorods were grown on Fluorine doped Tin Oxide (FTO) substrate using hydrothermal method. Morphological analysis shows growth of nanorod with more defects. The optical properties (UV-Vis spectroscopic and fluorescence spectrum) reviled the bandgap and quality of the grown nanorods. Poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT: PSS) is used to provide p-type contact over n-type ZnO nanorods to form

p-n junction. The photoconductivity study confirms the formation of a p-n junction with turn-on voltage of 0.3 V.

c0124

Photocatalytic cleaning of oil spill in sea water using indium sulfide nanoparticles

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An oil spill is the release of petroleum hydrocarbons into the marine environment. We report on the decomposition of oil spill using In2S3 photocatalyst. The In2S3 nanoparticles with In to S stoichiometry 1:1 were synthesized by homogenous precipitation method. The structural and optical properties of synthesized particles were studied using FTIR, BET and UV-Vis spectroscopy. The decomposition of oil spilled in sea water was achieved using 10 mg of In2S3 nanoparticles uniformly dispersed in the oil spill solution under the irradiation of visible light from 500 W Halogen lamp. Gas chromatography studies of the treated and untreated oil spill water confirms the decomposition of the crude oil compounds after 20 hrs of exposure to visible light.

c0126

Structural, Optical And Luminescent Studies In Calcium Silicate Doped With Ce

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Luminescence devices have become an essential part of our day-to-day life due to their wide variety of applications. They are used in various types of lamps, display panels, TVs, etc. Present work focuses on the modification of structural, morphological, luminescence, and optical properties of calcium silicate (CS) phosphor doped with 0.1% and 1% of Ce. The phase analysis confirms the formation of $CaSiO_3$ in the Wollastonite form with monoclinic crystal structure in CS and absence of variations in the crystal structure and the lattice parameter due to Ce doping. The agglomerated morphology, along with the absence of impurity atoms, are confirmed via Field Emission Scanning Electron Microscopy (FESEM) analysis along with Energy Dispersive X-ray spectroscopy (EDX). The photoluminescence studies confirm the predominant green colour in the emission spectrum of CS: Ce. Due to spin-orbit coupling, $5d\text{-}^2F_{5/2}$ and $5d\text{-}^2F_{7/2}$ transitions are noticed at 480nm and 502nm in CS: Ce. The bandgap measurement using UV-Visible spectroscopy confirms a bandgap of 4.92 eV in the CS host lattice. A concentration dependent reduction in the bandgap is identified with the Ce addition.

c0127

Effective and Environmental Friendly Lead-Free Tin Oxide Nanocomposite for X-Ray Shielding

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The present study is focused on the development of a lightweight, lead-free apron that can be used to shield low intensity radiation in medical imaging room. Sol-gel technique was used to produce SnO_2 nanoparticles (Nps). The synthesized Nps were coated on Rexine cloth with the help of Epoxy Resin. Similarly another sample was prepared using lead oxide micro

particles and this sample was taken as the reference to study the shielding effect of SnO_2 Nps. The X-ray diffraction (XRD) data was used to analyze the structure of the Nps. The crystallite size for prominent peak of the Nps was calculated around 31nm and found the crystal system was found to be tetragonal. The attenuation results of NC are compared with properties of lead oxide sample. The NC gives better attenuation results in low X-ray tube voltage.

c0128

Synthesis of Polyaniline-Crystalline Rubrene nanosystem by One-step Plasma Process: Exploring its Applicability in Broadband Optoelectronics by Plasmonic Functionalization

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In this report, the crystalline Rubrene and polymer material synthesis as well as the thin film deposition have been performed simultaneously in a unique plasma based single-step process. The applicability of the as-prepared thin film for development of a light responsive device in sandwich structure has been studied. We also demonstrate the plasmonic effect that occurs due to the incorporation of gold nanoparticles (Au NPs) in the prepared system. Significant enhancement in the spectral responsivity and specific detectivity of the device is observed after incorporating Au NPs in the organic semiconductor matrix.

c0129

Structural Attributes of High Capacity Resin by SEM

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Architectural and recurrence structure, spatial disposition of the resin and its accessibility w.r.t. metal ions and the related morphological attributes are investigated by SEM studies, where the fine channels, trammels, glimpses of ups and downs, corrugated structure have been found out by diagnosis of the spectroscopic view by microscopy such as optical microscopy (OM), scanning electron microscopy (SEM), etc.

c0131

Optical and Electrical Properties of Sn Doped TiO_2 Nanoparticles

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In this work we successfully doped Sn in the place of Ti in an anatase and rutile structure from 0.1% to 0.5%. Scherrer formula confirms the average crystallite size from 92-40nm. SEM images shows the reduction in the size and tending towards spherical in nature with average particle size from 110-40nm. Pellet form of these samples were studied in the frequency range from 1MHz – 10MHz, which shows the ε' more in the lower frequency range for the particle size of 67nm at 1MHz it decreases instantly then saturates with increase in frequency due to charge carriers, with hopping conduction is prominent at this region. σ_{ac} increases with increase in frequency, at 1MHz σ_{ac} maximum for average particle size and it decreases with decrease in particle size due to hopping conduction become more prominent.

c0132

Synthesis of SnS Nanoparticles by Homogeneous Precipitation Technique by Varying Temperature

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This work investigates the formation of tin sulphide nanoparticles using homogeneous precipitation technique by varying the initial reaction temperature from 50 ^{0}C to 300 ^{0}C. The molarities of reactants (0.6M of $SnCl_2$ and 0.1 M of TAA) and time for heat treatment (2hrs) kept fixed throughout in the reaction. The prepared samples were characterized using UV-Visible absorption spectroscopy and X-Ray diffraction (XRD). Samples, synthesized under temperatures 100^{0}C -200^{0}C shows an increase in their band gap (from 1.88 eV to 3.19 eV) due to decrease in particle size. For 250^{0}C and 300^{0}C band gap decreases, this attributed to formation of the secondary phases. The structural properties and composition of samples were studied using XRD pattern and shows a prominent orientation along (111) plane which matches with orthorhombic phase of SnS. The formation of secondary phases when treated at higher temperatures is in confirmed from the peaks corresponding to SnS_2 and Sn_2S_3particles.

c0133

Effect of Temperature on the Synthesis of β-In_2S_3 Quantum Dots in Perfluorinated Ion Exchange Membrane

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Semiconductor quantum dots have found extensive industrial application due to their unique physical and chemical properties. In this study, β-In_2S_3 quantum dots were synthesized in perfluorinated ion exchange membrane (Nafion 117) through a simple wet chemical method at different temperatures from 50^{0}C to 90^{0}C and the effect of temperature in the process was studied. The band gap energy calculated from the UV-Vis absorbance shows a blue shift which confirms quantum confinement. The photocatalytic activity of this membrane under visible-light irradiation was investigated considering the degradation of organic matter in sea-water. The results show reduction of organic matter and also the effective removal of micro-organisms like *e-coli* and *coliform bacteria* from sea water. The band gap energy of the membrane is found to reduce after each use as a photocatalyst.

c0135

Spin Coating Induced β-Phase in Ultrathin PVDF film for MEMS Based Devices

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Poly(vinylidene fluoride) (PVDF) thin films with controllable thickness and surface roughness are prepared by heat controlled spin-coating technique. It has been realized that roughness down to 6 nm with 76% yield of ferroelectric β-phase is possible to achieve that exhibits superior nanoscale piezoelectric coefficient (d33) -24 pC/N. In addition, long retention of ferroelectric phase switching behaviour is also observed. Ferroelectric switching associated to phase and generated strain vs. applied voltage hysteresis curves indicate the potential application of PVDF ultrathin film in MEMS based electromechanicalsensors, actuators, and non-volatile memories.

c0136
Morphology and Molecular Orientation of Nanofibers in Electrospinning and it's Piezoelectric Nanogenerator
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The electrospinning parameters play a critical role to obtain a particular morphology and prominent electroactive phase of the PVDF in nanofibers, majorly governed by Taylor cone formation, viscosity of the polymer, flow rate and relative humidity. Polarization dependent vibrational spectroscopy technique is one of conclusive way to study the dynamics of the molecular dipoles nanofibers upon altering the polarization of IR light at particular angle. The fabricated Piezoelectric nanogenerator showed max open circuit voltage (V_{OC}) of ~2.8 V and max short-circuit current (I_{SC}) of ~ 48 nA.

c0138
Synthesis and Magnetic Properties of Unusual Hexagonal Nickel Nanostructures
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In this study, we report the synthesis and processing of hexagonal closed packed nickel (HCP-Ni) via the cost-effective and scalable polyol method. The reaction is carried out with stoichiometric amount of Nickel acetate, Polyvinylpyrrolidone, which have been refluxed in Ethylene glycol (EG-Ni) and Di-ethylene glycol (DEG-Ni), for 3hrs. DEG was chosen as an appropriate solvent that yields larger percentages of HCP-Ni in addition to FCC-Ni. Further processing of colloids improved the yield of HCP-Ni in the mixed powder made from DEG. The magnetic studies of synthesized nanostructures are also investigated.

c0139
Phase Evolution in Sol-Gel Synthesized Barium Titanate Ceramics
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In this work sol-gel synthesized BaTiO3 ceramics were studied for phase formation using X-ray diffraction. The effect of increase in calcination temperature was analyzed to see how BaTiO3 crystallizes initially into cubic phase and then into tetragonal phase. Lower calcination temperatures below 500°C were not able to provide enough thermal energy

required for formation of these ceramics. However, temperatures above 800°C lead to formation phase pure BaTiO3. At sintering temperature of 1350°C, these ceramics predominantly crystallize into tetragonal phase.

c0140

Synthesis And Characterization Of Lanthanum Modified Tungsten Trioxide And Its Efficient Antibacterial Performance

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Present work is focused on the investigations of La doped WO3 nanoparticles for their potentials applications in the field of antibacterial activity towards Escherichia coli (E. Coli) bacteria. Different doping concentration of Lanthanum (2%, 4%, 6% and 8%) in WO3 was studied. The prepared samples were characterized by X-Ray Diffractometer (XRD), Fourier Transform Infrared Spectroscopy (FTIR). Antibacterial activity towards E. Coli bacteria were studied at different concentrations using La incorporated WO3 photocatalyst.

c0141

Impedance Spectroscopy of La doped BiFeO3 Nanoparticles

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We investigated the influence of La substitutional ions on the impedance spectroscopy properties of bismuth ferrite (BiFeO3). Our compositions of 1.05Bi1-xLaxFeO3 (x =0 to 5%) nanoparticles (NPs) have synthesized by sol-gel method. An increase in the dealing parameters of the rest time observed by electric analysis was established up to 5% La doped BiFeO3 NPs. The impedance spectroscopy of La doped BFO is fitted with the R(C(R(QR)))(CR) model using cole–cole plots. It was found that a La-content of 1.05Bi0.95La0.05FeO3 generated extra charged space that can across the threshold to initiate conduction due to these multiferroic materials.

c0144

Surface Plasmon Tunability of Green Synthesized Gold Nanoparticle Using Plasma Liquid Interaction

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High-quality and surfactant-free nanomaterial synthesis using Plasma – Liquid Interaction (PLI) technique is a rapidly growing interdisciplinary field in the interface between the plasma and material science. It offers single-step, rapid and large scale synthesis of nanomaterial of different shapes and sizes by simply controlling the physical as well as chemical parameters. One of the major advantage of this process is that it does not require any toxic reducing or stabilizing agent, due to which the process can be considered as a green process. This report involves the development of a plasma – liquid reactor for the fabrication of gold nanoparticles (Au NPs) of different sizes using PLI by controlling a physical and a chemical parameter that significantly influences the optical properties of Au NPs. OES spectra confirm the reactive species generated in the plasma zone.

c0146

Effect of Co-Doping (Y, Co) on Structural and Optical Properties of $LaFeO_3$

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The structural and optical properties of nanocrystalline $La_{0.7}Y_{0.3}Fe_{0.7}Co_{0.3}O_3$ sample, synthesized by sol-gel auto-combustion route, have been studied. The X-ray diffraction pattern shows that the sample was successfully formed in single phase perovskite structure. The value of tolerance factor (< 1) indicates the distortion and deviation from ideal perovskite structure. The Raman analysis reveals that the structure of the prepared sample is consistent with that of $LaFeO_3$ orthorhombic perovskite structure with *Pbnm* space group. Raman analysis reveals the compressive stress in the material. The Energy bandgap (E_g) as determined using Tauc's relation is found to be 2.93 eV.

c0149

Photodegradation of Methyl Orange Dye by Hydrothermally Grown CdS Nanoparticles

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This paper focuses on the synthesis of CdS nanoparticles under hydrothermal route, studying their structural, morphological properties and photo degradation studies on the dye of methyl orange. Now day's methyl orange widely used dye in textile industry. For pollution free environment dye degradation is a one of the major component. From XRD studies CdS nanoparticles shows hexagonal phase with crystal lattice size of 12 nm and exhibiting the spherical spheres type morphology. A 400 watt halogen lamp is used to irradiate the CdS added dye solution to imitate the sunlight. For 100 ppm pure dye is on 464 nm showing the absorption value as 0.6235 respectively. This indicates that the absorption value is directly proportional to concentration. the concentration increases intensity of the peak increases. As the concentration of the dye and Irradiation Time increases the degradation percentage increases. We can also see the red shift for the 2nd peak after adding the nanoparticles. The peak shifted towards 460nm from 464nm in UV-VIS analysis. Which does mean the dye is getting degraded and colour is fading. By which we can conclude that CdS nanoparticles are acting as photocatalyst and breaking the dye complex structures into simpler compounds by pseudo first order kinetics.

c0150

Synthesis Of ZnO Nanoparticles By Sol -gel and Co-precipitation Methods & Comparison Of Their Structural Properties.

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Present work demonstrates the synthesis of Zinc oxide nanoparticles by co-precipitation and sol-gel methods. The prepared ZnO nanoparticls are further characterized by using X-ray diffraction technique. It has been observed from the X-ray diffraction data that both the variants exhibits hexagonal wurtzite structure. The particle size calculated for ZnO prepared by sol-gel is 29.90 nm and for ZnO prepared by co-precipitation is 20.66 nm. Furthermore it is found that the unit cell volume of ZnO nanoparticles prepared by sol-gel is smaller than the unit cell volume of ZnO sample prepared by co-precipitation method.

c0151

Structural and morphological analysis of nico2o4 prepared by hydrothermal technique

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In the present work, NiCo2O4 is prepared by hydrothermal method and its structural, morphological and electrochemical characteristics are analysed. From XRD, the average crystallite size changes from 17 to 9 nm when the nickel nitrate and cobalt nitrate ratio varies from (1:1, 1:2, 2:1). The surface morphology of the samples is imaged by a Field emission - scanning electron microscope. Most of the prepared particles are spherical in shape. As increases the Ni and Co concentration, the particles growth are from irregular to spherical in shape. Electrochemical studies is also carried out for the prepared samples.

c0152

Synthesizing Silver Nitrate Nanocrystals from Rapidly Evaporating Microdroplets

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Silver nitrate nanocrystals had been synthesized in large-scale by spray-drying an aqueous colloidal solution containing silver nitrate, polymer polyvinylpyrrolidone and ethylene glycol. The formation of silver nitrate nanocrystals had been confirmed using electron microscopy and x-ray diffraction. A small fraction of silver nanoparticles also formed during spray drying as confirmed by UV-Vis spectroscopy. Upon heat treatment, these silver nitrate nanocrystals reduced to silver nanocrystals as confirmed from x-ray diffraction and transmission electron microscopy. Thus, spray-drying can be used as an efficient and facile technique for large-scale production of silver nitrate and silver nanocrystals for various applications.

d: EXPERIMENTAL TECHNIQUES AND DEVICES

d0002

Charge Injection Mechanism in Semiconductor Memory Devices

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Charge injection mechanism has been investigated in the two nonvolatile, semiconductor flash memory devices using a high-speed capacitance-voltage (HSCV) measurement system. The capacitance measurement process is fast in terms of measurement speed that it completes capturing the entire CV curve in less than 10 µs. The system is capable of generating sequential pulsing sessions to inject the charges into the defect states and simultaneously measuring the HSCV curve. A continuous shift of the HSCV curve, as well as flatband voltage (V_{FB}) owing to injection of the charges into two terminal flash memory devices. The program state of memory devices is achieved due to the saturation of flatband voltage shift (ΔV_{FB}). The continuous charge injection helps to saturate the ΔV_{FB}. This mechanism confirms the availability of program and erase memory state in the semiconductor flash memory devices.

d0003

Effect of Gravity on the Vertically Flowing Down Water Jets

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A clean water jet flowing under gravity is allowed to impinge on the surface of deep water reservoir contaminated with tide detergent, a fluid pipe is formed on the jet extend up to some height from the surface of reservoir. The capillary waves appeared above the fluid pipe and the bulbous below which join the fluid pipe to the reservoir. We performed the experiment to measure the fluid pipe height H at various jet length L, flow rate Q, nozzle inner radius r_0 and concentration c = 5 mg cm^{-3} of tide-detergent-water solutions in order to study the effect of acceleration due to gravity on the vertically flowing down water jets. We compare our experimental values of dimensionless fluid pipe height $\frac{H}{aRe}$ with the values of approximate expression using $f_1 = \frac{2.73}{We_d{}^2}$ and $f_2 = \frac{2.73}{We_d{}^2}\left(1+\frac{25.1}{We_d}+\frac{0.879}{SWe_d{}^2}\right)^{-1}$ deduced by Hancock and Bush.

d0004

A GUI-based 2D-SAXS Data Analysis Software for Study of Anisotropic Structure in Mesoscopic Length-scale

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A graphical user interface based software package, named 'SAXS2D' has been developed for analysis of 2D small-angle X-ray scattering (SAXS) data. The software has been tailor-made for handling a large amount of SAXS data of the newly installed SAXS beamline of Indus-2 synchrotron both in interactive and batch mode. The unique feature of this Python language based software package is to analyze 2D-SAXS data, especially the anisotropic 2D-scattering patterns to reveal orientated and/or anisotropic structure in mesoscopic length scale. To demonstrate the performance of the software, the structural analysis of anisotropic pores distribution present in a shale-rock sample has been presented

d0007

Modeling and Performance Analysis of Optical Microring Resonator for Chemical Sensing

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The progress of technology from electronics to photonics is now evident more than ever, due to the ever increasing demands of faster and miniaturized technological gadgets; especially sensors. Several efforts have been made to optimize the selection of materials for such photonicapplications. In this work, we have designed and simulated optical micro-ring resonators with different optical materials for their use as an efficient chemical and biological detector. We modeled an optical ring resonator with dimensions of the waveguides as small as 200nm. Using this model, we studied the absorbance, reflectance and transmittance of resonator for materials like silicon nitride, silicon-on-insulator (SOI). We also conducted a study to analyze the behavior of device when exposed to ethanol on the sensor surface. After modifying sensing surface for ethanol sensing we observed a shift in resonating wavelength. For SOI based resonator the wavelength shift was 4.05 nm and for silicon nitride based resonator the shift 10.03 nm.The modeled device had a quality factor of 2129 and 556; the finesse was obtained to be 48 and 12 for SOI and Silicon Nitride based optical microring resonator structure respectively; the details of which will be discussed in this presentation.

d0008

Curved Structured 3D Printed Flexible Triboelectric Nanogenerator

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3D printing is a versatile tool to fabricate any structure of desired shape and size, as a result an attempt has been taken to fabricate the tribo electric nanogenerator (TENG). We have prepared a curved structured TENG that exhibits superior flexibility and excellent mechanical energy harvesting capabilities. It is also expected to integrate with various parts of the body to monitor diverse human activities.

d0009

Detector Performance Study for Cargo Scanning Applications using Monte Carlo Simulations

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Cadmium tungstate (CdWO4) scintillator coupled to silicon PIN photodiode was investigated as a detector for Cargo Scanning applications for 6 MeV LINAC polychromatic X-ray spectrum. Monte Carlo (MC) simulation study was carried out for the generation and transportation of 6 MeV X-ray spectrum and to study energy deposition in CdWO4 crystal. The penetration of 6 MeV X-rays through various thickness of steel was theoretically estimated. Images of stainless steel (SS) plates behind thick SS blocks were generated with the simulation data.

d0010

Photoluminescence Properties of Orange Red Emitting $LiSrP_3O_9:Sm^{3+}$ Phosphor

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The Combustion method was used to synthesize the orange-red light emitting $LiSrP_3O_9:xSm^{3+}$ (x = 1 mol%) phosphor. Powder X-ray Diffraction analysis was used to confirm the phase of the prepared $LiSrP_3O_9:Sm^{3+}$ phosphor and photoluminescence (PL) properties were investigated under ultraviolet (UV) excitation (300-450 nm). The wavelengths 595 nm and 398 nm were used to record the excitation and emission spectra of the prepared phosphor. The emission spectra of $LiSrP_3O_9:Sm^{3+}$ phosphors consist of series of sharp lines centered at 559 nm, 595 nm and 641 nm corresponding to $^4G_{5/2} \rightarrow {}^6H_{5/2}$, $^4G_{5/2} \rightarrow {}^6H_{7/2}$ and $^4G_{5/2} \rightarrow {}^6H_{9/2}$ transitions of Sm^{3+} ion respectively. The CIE (Commission International de l'Eclairage) coordinates were calculated and determined to be x = 0.58, y = 0.42. Therefore, the $LiSrP_3O_9:Sm^{3+}$ phosphor is a promising material for use in wLEDs.

d0011

Transport Measurements Set Up To Probe Single Atomic/Molecular Junction At Room Temperature

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Understanding the transport at the atomic limit (single atom or molecule) is the prerequisite to explore the future generation nano-electronic applications. Among various experimental procedure, mechanically controllable break junction (MCBJ) is one of the well accepted experimental techniques to study and understand the atomic or molecular scale devices. In the present work, we demonstrate the fabrication and characterization of a gold atomic contact and 4, 4' bipyridine single molecular junction between gold electrodes using a homemade MCBJ experimental set up.

d0012

Deep Red Emitting Eu3+ Activated Sr3B2O6 Phosphor for White Light Emitting Diodes

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The Sr3B2O6:xEu3+ phosphors were synthesized by the combustion technique. The structural and luminescent properties of the material had been explored using powder X-ray diffraction (XRD) and Photoluminescence (PL), respectively. The powder XRD results showed the formation of single-phase Sr3B2O6:xEu3+ phosphors with rhombohedral crystal system and space group R-3c. PL results showed that under 394 nm excitation, the prepared Sr3B2O6:xEu3+ phosphors give four characteristic emissions due to the 4f-4f transitions. i.e. 5D0 → 7FJ (J = 1,2,3,4). The strongest emission peak at 614 nm is due to 5D0 → 7F2 transitions which give intense red emission. The CIE coordinates for Sr3B2O6:xEu3+ was (x = 0.65, y = 0.35) which falls in the red region of the horseshoe gamut with a color purityof 99.3%. The result shows that Sr3B2O6:xEu3+ phosphor can be used in blue chips-based white-LED's

d0013

Biofilm Thickness Measurement by Doppler Optical Coherence Tomography (D-OCT) and Speckle Interferometry

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Optical coherence tomography (OCT) utilizes low coherent light source to capture two and three-dimensional images of biological tissues with micrometer resolution. In addition to morphology, the approach has experienced a number of developments aimed at assessing functional features of the tissue. We present our estimate of the thickness of a biofilm as measured by speckle interferometry technique and also by using our locally developed Doppler OCT (D-OCT) system. The results are comparable with those obtained from SEM cross sectional images and are found to be in close agreement

d0015

Thermographic Studies of $CaSr_2(PO_4)_2:Sm^{3+}$Phosphor for High Temperature Sensing

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This work presents the synthesis of $CaSr_2(PO_4)_2:Sm^{3+}$ phosphors prepared via solution combustion method and the photoluminescence (PL) properties had been investigated to explore its potential application in luminescence thermometry. The PL studies reveal that the phosphor had a strong absorption in the ultraviolet region and sharp emission peaks at 562 nm, 600 nm, 645 nm and 706 nm due to the 4f-4f transition of the Sm^{3+} ions. Further, temperature dependent PL studies were done to examine the phosphor for thermometry application. The fluorescence intensity ratios (FIRs) between the emissions of the Sm^{3+}: $^4G_{5/2} \rightarrow {}^6H_{5/2}$ (564 nm) to the Sm^{3+}: $^4G_{5/2} \rightarrow {}^6H_{7/2}$ (600 nm) were calculated as a function of temperature in the range of 323-473K. The sensitivity obtained had a maximum value of 0.00116 K^{-1} indicating that the prepared phosphor is a promising candidate for optical thermometry.

d0016

Efficiency improvement of heat pipe with Graphene/R-410a working fluid

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This paper aims to improve the thermal eficiency of heat pipe (HP) by using graphene / R 410a nanorefrigerant. In this study graphene nanoplatelets (0.75% volume concentration) with R 410a refrigerant is used as a working fluid. Different heat power (60W, 80W) and inclination angles (00,450,900) are implemented to HP in order to validate the thermal resistance, thermal efficiency. Based on this study, nanorefrigerants enhance thermal efficiency, at the same time decrease thermal resistance. Thus the study suggests that HP with nanorefrigerants are well suitable for cooling techniques in all industries.

d0017

Synthesis Of Strontium/Barium Titanate ($(Sr/Ba)TiO_3$) Nanoparticles Using New Sol-gel Technique And Study Of Their Optical Properties

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Strontium/barium titanate ((Sr/Ba)TiO_3) nanoparticles have been successfully synthesized by employing a new, facile, easy and cost-effective sol-gel technique using Titanium isopropoxide (TIP), nitrates of Sr/Ba and ethanol and water as solvent. The structures of the prepared samples were confirmed using XRD. It revealed the formation of pure cubic phase of $SrTiO_3$ and tetragonal phase of $BaTiO_3$ after calcining the sample at 800^0C for 5hrs and then 1200^0C for 10hrs. The optical properties of the synthesized (Sr/Ba)TiO_3were demonstrated using FTIR and UV-Visible spectroscopy. The band gap of $SrTiO_3$ and $BaTiO_3$ was 3.08 and 3.26 respectively. The band gap of $SrTiO_3$ is in the visible region which makes it a potential candidate for photocatalytic applications.

d0018

Design and commissioning of neutron time-of-flight spectrometer at Dhruva reactor

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The neutron time-of-flight spectrometer commissioned recently at Dhruva reactor provides high throughput in terms of higher neutron flux at the sample position and a large solid angle of detector coverage. This instrument incorporates focusing monochromator, neutron Fermi chopper, an array of linear position sensitive detectors, and position encoding and time-read out electronics. Background scattering has been minimized with adequate shielding of all components. Comparison of the measured data with the results of Monte Carlo simulations is demonstrated.

d0019

Microstrip Line Based Complementary Resonant Structure For Dielectric Characterization

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In this work, a complementary resonant structure etched on the ground plane of a microstrip line is proposed for characterizing dielectric materials. The resonant sensor is designed to operate in S-band (2 – 4 GHz). The sensor is designed in an electromagnetic simulator to generate its transmission response, electric and magnetic field maps. Numerical model of the sensor is established to determine the electric permittivity of dielectric samples. The sensor is fabricated on a soft microwave laminate using a rapid photolithography technique. The electric permittivity values of wood, Teflon, and RT/duroid® 5880LZ are determined by using the sensor. The permittivity values are found to be consistent with those available in the literature.

d0020

Role of Natural Dye in Photovoltaic Performance of Dye Sensitized Solar Cell

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Investigating cost-effective alternatives to organic dyes for use in dye-sensitized solar cells (DSSC) could help to lower the overall cost of the devices.This manuscript deals with optical and structural properties of novel natural dye extracted from harda fruit.The optical absorbance, emission and functional group of natural dye has been studied using UV-Vis. spectroscopy, photoluminescence and Fourier transform infrared (FTIR), respectively. The DSSC has been fabricated using natural dye as photo-sensitizer and studied their photovoltaic performance. The power conversion efficiency (PCE) for DSSC has been achieved up to 2.7%. Although the use of natural dye in DSSC improved the better short-circuit current density (Jsc) and open-circuit voltage (Voc).Understanding these fundamental properties of natural dye could pave the way for the development of natural dyes based solar cells.

d0021

Automated Thermally Stimulated Current Measurement Setup for Characterizing Photovoltaic Materials

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Investigating the trap distribution in semiconducting materials is very important because of its influence on various optoelectronic properties and on the efficiency of the fabricated devices. Thermally stimulated current (TSC) experiment is a versatile technique for investigating the electronic trap states in semiconducting materials. This work reports the development of a LabVIEW based automated TSC experimental setup with sub-pA current sensitivity. The developed setup is used to obtain trap activation energies of Poly[2-methoxy-5-(3',7'-dimethyloctyloxy)-1,4-phenyle and Methyl Ammonium Lead Iodide perovskite materials.

d0022

XANES study of gamma irradiated $CaSO_4$:Dy for dosimetry

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$CaSO_4$:Dy thermoluminescence (TL) dosimeter has a linear dose response up to 30 Gy using the TL dosimetry technique. X-ray Absorption Near Edge Structure (XANES) technique is

explored to extend its useful dose range to higher gamma dose. The present study is carried out up to gamma dose of 5 kGy and the XANES results are presented. The study indicates that the XANES technique provides a linear response up to 1 kGy.

d0023

Carbon-nanomaterial-based Ternary Composite as Photoactive Layer

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Here, we prepared the reduced graphene oxide (rGO): carbon nanotubes (CNTs): Buckminsterfullerene (C60) based all carbon ternary composites with the aim to study the optoelectronic properties, in order to utilize them in the photoactive layer of optoelectronic devices. The facile solution processing method has been used to prepare the composite thin film. Field emission scanning electron microscopy analysis validates the development of ternary composite. The as-prepared composites were used to fabricate the two kinds of device, one comprising the photoactive layer made by composites of rGO, C60, and single-walled type CNTs and in another device, everything was the same except the single-walled CNTs were replaced by multiwalled type CNTs. The device containing multiwalled CNTs demonstrated greater optoelectronic performance compared to that of the device comprising single-walled CNTs. The lower ideality factor of the multiwalled CNTs composite-based device suggests better interface quality, therefore better interface quality might be attributed to the superior optoelectronic performance.

d0024

Measurement of Neutron Fluxes Incident on Neutron Transmutation Doped Si Samples Irradiated in Apsara-U Core

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Irradiations of Neutron Transmutation Doped-Silicon (NTD-Si) samples were carried out at core positions of newly commissioned Apsara-U (Apsara-Upgraded) reactor at BARC. This was part of feasibility studies carried out for NTD-Si production at Apsara-U. For proper characterisation of the irradiated NTD-Si samples, it is very important for continuous monitoring of neutron fluxes at the irradiation locations. Using thermal and fast neutron activation monitors, neutron fluxes were measured during NTD-Si irradiations at two core positions (G4 and H7) of the reactor. The fluence seen by the sample, thus estimated, were further utilised for resistivity characterisation of the irradiated Si-samples

d0025

Luminescence investigations on low energy He^+ ion irradiated ZrO_2

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In the present work, monoclinic zirconia was irradiated with 100 keV He^+ ions and during ion irradiation, the ionoluminescence experiments were carried out with the ion fluence interval of ~1.49×10^{15} ions/cm^2. Photoluminescence (PL) and Raman scattering measurements were carried out before and after ion irradiation. Raman scattering results reveals that, the structure of zirconia is monoclinic form, and upon ion irradiation, slight shift in the Raman mode along with broadening is observed, however, monoclinic to tetragonal phase transformation was not observed. Ionoluminescence and photoluminescence experiments are consistent, with defect cluster formation and its growth, the intensity of luminescence signal is quenched.

d0026

Diffusivity measurement in Zr-2.5%Nb alloy using Neutron Radiography

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Zirconium alloys have long been used in nuclear industry owing to their special properties. They however suffer from the problem of hydrogen embrittlement which results in reduced service life and issues. Hydrogen estimation in Zr-alloys is an area long studied using several techniques. Neutron radiography offers the advantage of being a nondestructive technique which provides bulk hydrogen information in a short span. Apart from hydrogen concentration study of its redistribution under different types of gradients like stress, temperature and concentration is especially important. Here we present evaluation of the diffusivity value of hydrogen in Zr-2.5%Nb alloy at 673K. Studies have been carried out on samples from pressure tube which were pre-charged electrolytically and annealed for a definite time at said temperature to generate a diffusion profile.

d0028

EOS and Mechanical Properties of Cu-Ti Alloy under Dynamic Loading

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The shock compression study in the pressure range of 4.92GPa- 14.28GPa has been conducted on Cu-5%Ti alloy via plate-impact experiments using single-stage gas-gun facility. The experiments were designed to create both compressive and tensile stresses in the sample so as to measure mechanical strength properties such as Hugoniot elastic limit (HEL) and spall strength apart from determining Hugoniot data. From the free-surface velocity profiles of the target measured by Photon Doppler velocimeter (PDV), the HEL and spall strength is determined to be in the range 1.32GPa-1.76GPa at strain rates 3.56x104-10.56x104 s-1and 2.12GPa-2.34GPa at strain rates of 2.33x104- 4.05x104 s-1, respectively. The comparison of the generated Hugoniot data of this alloy with pure copper indicates that the addition of 5%Ti slightly influence the EOS. However, the dynamic strength properties, i.e., HEL and spall strength differed significantly from that of pure Cu.

d0031

Photoluminescence Study of Eu^{3+} Activated Ca_2CeNbO_6: Red Emitting Double Perovskite Phosphor for LED Application

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Eu3+ doped Ca2CeNbO6double perovskite phosphors were synthesized via high temperature combustion method, in which urea is taken as a flux. The synthesized phosphors have polycrystalline structure with homogeneous particle size. The structural and crystalline parameters have been determined from the x-ray diffraction patterns. Prepared phosphors have orthorhombic structure. It is observed that the crystallite size increases with increasing doping concentration of Eu3+. The photoluminescence (PL) properties of the phosphors have been investigated using 467nm excitation wavelength. The phosphor shows high intense red emission at 614nm when phosphor was excited with 467nm wavelength. Having intense red emission due to the characteristic electric dipole and magnetic dipole transition of Eu^{3+} ion at 467nm excitation would signify its LED application.

d0032
Metal Nitride Heterostructure for UV-B Photodetection
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Interband transition generated carriers of plasmonic nanostructure offer a new scope for the detection ofhigher energy photons. In this report, an effort has been made to utilize the interband carriers of titanium nitride (TiN_x) for UV detection by fabricating a metal-semiconductor heterostructure (TiN_x/ TaN_x). The active components of the device are synthesized by pulse DC magnetron sputtering technique, and subsequent photoelectrical characterization confirms the generation of photocurrent by UV light. The maximum performance of the detector is found to be in UV-B region where $X_5 \rightarrow X_2$ transition(3.9 eV) of TiN_xtakes place. Theexcitonic carriers of semiconducting tantalum nitride (TaN_x) also contributes and enhanced the overall performance in this region.

d0033
Magnetodielectric $Ni_{0.5}Zn_{0.3}Co_{0.2}Fe_2O_4$ and $SrFe_{12}O_{19}$ Composite for Ferrite Resonator Antenna Applications
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A conventional solid-state sintering method is adopted for the fabrication of x Ni0.5Zn0.3Co0.2Fe2O4−(1−x) SrFe12O19 composite with x = 0.5, with appreciable density and their broadband electromagnetic properties were deciphered. X-ray diffraction analysis revealed the presence of Ni0.5Zn0.3Co0.2Fe2O4 (NZCFO) and SrFe12O19 (SFO) phases in the composite along with minor impurity phases. The composite possesses a stable real permittivity of 8.9, dielectric loss in the order of 10−2, permeability greater than 2 and magnetic loss tangent in the order of 10−1 in the broadband region. A ferrite resonator antenna based on NZCFO-SFO composite has been simulated and fabricated. The fabricated resonator antenna operates at 13.4 GHz presented an exceptional return loss of -28.5 dB with a wide impedance bandwidth of 1.7 GHz.

d0035
MEMS based pressure sensor for detection of negative pressure wave in subsea pipelines
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Design analysis and simulation of a MEMS based capacitive pressure sensor for detection of a negative pressure wave (NPW) has been presented for leak detection in subsea pipelines. A capacitive pressure sensor measures the change in pressure through a calibrated circuit due to displacement of the membrane. Capacitive pressure sensor involves two coupled physics, namely Electrostatics and Solid mechanics. COMSOL Multiphysics was used to simulate the sensor behavior under various conditions. A negative pressure wave, modeled in MATLAB, was imported as an input load to study the change in impedance and its sensitivity to different parameters. The parameters chosen for sensitivity analysis were (a) the material of the capacitor membrane and (b) the gas-filled in the cavity. Simulation study showed that the maximum displacement occurred at the center of the sensor membrane and reduced radially outwards; also a change in the capacitance due to the change in membrane material is also observed. While the same deflection and capacitance was observed when the cavity was filled with air and noble gases, there was improved total capacitance when the cavity was filled with Nitrogen. We conclude that a change in the dielectric material of the cavity and membrane material has a positive effect on the sensitivity of the sensor.

d0036

Niobium Doped Bismuth Titanate Ceramic Piezo-Elements for High Temperature Transducer Application

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Polycrystalline ceramics of bismuth titanate $Bi_4Ti_3O_{12}$ (BIT) doped with 3 mol% Nb were synthesizedby solid state sintering method. Synthesis process was optimized to get phase pure material. Piezoelectric properties of this material were studied. Sintered pelletized BIT discs were polled and used as an active piezo element. In initial experiments these BIT discs were tested for ultrasonic transducer application using pulse echo method. Results of study indicate that prepared piezo ceramic has potential to be used for high temperature transducer applications.

d0039

Structural Characterization of Pure Monazite Phase in $LaPO_4$

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We report Rietveld refined data of X-ray diffraction experiments performed on monazite $LaPO_4$, which is considered to be a potential host material for immobilization of metallic actinides produced as nuclear waste products. The sample was synthesized via solid state reaction method with starting material as La_2O_3 and $(NH_4)_2HPO_4$ at elevated temperature of 1550°C followed by sintering in air atmosphere. X-Ray diffraction measurements revealed the phase purity and crystallinity of sample. Energy dispersive X-ray analysis technique was used to determine any chemical impurity present and elemental composition. The sample was found to be in monoclinic crystal structure with space group number 14 and symmetry $P2_1/n$ with the lattice parameters close to the expected ones (standard bulk). Present studies

would be used as a basis for further characterization of this material to understand its suitability as a host for waste immobilization.

d0042

G Phonon Mode Splitting in Doped Bilayer Graphene Probed by in-situ Transport Measurement and Raman Spectroscopy

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Two dimensional material like graphene, TMDC's have shown a lot of promises due to their excellent electrical and optical properties. Graphene devices fabricated so far relied on lithographic techniques which always leave an un-intentional residue on the graphene surface. Here, we have created a bilayer graphene device avoiding the conventional lithographic procedure by transferring the graphene layer directly on top of the metal electrodes. We tune the carrier density by the application of an electrolyte top gate, and a high doping level (~ $10^{13}/cm^2$)can be accessed due to the formation of a nanometer-thick Debye layer. We performed in-situ Raman spectroscopy by varying the carrier concentration. A prominent blue shift of thecharacteristic G peak was noticed with increasingcarrier concentration, originating possibly due to enhanced electron-phonon interaction. Moreover, we observed a splitting of the G peak at higher doping concentration, may arise due to mixing of symmetric andantisymmetric modes by breaking the layer symmetry of the bilayer graphene.

d0043

High Efficiency, Zero Dead Space, Square Cathode Neutron Detector For Triple Axis Spectrometer

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Neutron scattering instrument with optimized detectors enhances the instrument through put. Position sensitive detectors show considerable gain in beam time utilization, whereas few experiments such as Triple Axis Spectrometer need point detector in step scan mode for recording the neutron intensity in variable (Q,ω) space. Use of focusing monochromator, planar beam monitor for integral beam intensity counting and efficient neutron detector with zero dead space and square cross section area are of advantage. Neutron efficiency, beam interception area and shielding volume put constraints on the overall design of the detector. It is essential to have compact detector with high neutron detection efficiency, indicating position in(Q,ω) space and high beam interception. Square cross section neutron counting detector is designed and developed for use at Triple Axis Spectrometer. The present detector also gives the advantage of reduced shielding weight on movable arm of detector.

d0044

Synthesis and characterisation of $GdTaO_4$ using XRD, Raman, and first principles calculation

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In recent times, the family of Ternary oxides RBO_4 (R = Gd, Eu, Dy and B = Nb, Ta) has drawn special attention because of their potential application in field of solid-state fuel cells, scintillating crystals, anti-laser radiation area and so on. We have synthesized polycrystalline $GdTaO_4$ by solid state reaction method and characterized same compound by using XRD, and Raman techniques. First principles calculations have been performed using Quantum espresso and the structural parameters and Raman mode frequencies, obtained from DFT calculations corroborates well with our experimental findings.

d0045

Internal Field Nuclear Magnetic Resonance: Versatile tool to Estimate the Fe^{3+} ions concentration in Ferrites

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To determine the concentration of Fe3+ ions in the ferrimagnetic materials there are only few limited tools: one such is Internal Field Nuclear Magnetic Resonance (IFNMR). To estimate the concentration we have chosen two ferrimagnetic materials Nickel ferrite and Lithium Ferrite. The determined concentration of Fe3+ ions is in good agreement with the existing tools such as XRD and Mössbauer etc.

d0046

Development of In-situ X-ray Imaging and µ-CT facility for Sample Studies Under Tensile/Compressive Load Conditions

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X-Ray micro tomography is versatile tool for study of properties of materials like density, micro structure etc. There is great demand in studies related to change in the properties of materials under various loading conditions (such as mechanical stress and temperature). An In-Situ X-Ray imaging and u-CT facility with compression and tensile loading stage have been developed at imaging beamline Indus – 2. This facility allows study of material micro-structures under compression and tensile load conditions. This papers describes in details about the facility developed.

e: GLASSES AND AMORPHOUS SYSTEMS

e0003

Characterization of Polystyrene based Plastic Scintillator for Neutron Detection Applications

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A polystyrene based plastic scintillator of 4.5 cm diameter and 2.5 cm length doped with 2,5-diphenyloxazole (PPO) and 1,4-bis[2-(phenyloxazolyl)]-benzene (POPOP) was synthesized using thermal polymerization reaction in the temperature range of 30 to 120°C. The radioluminescence measurement of the synthesized sample exhibited a very strong emission band in the wavelength range from 320 to 450 nm with a peak maximum at 420 nm for different voltages.The fast scintillation decay time of the fabricated plastic scintillator was investigated using γ-rays from ^{137}Cs radiation source. Pulse height spectra were recorded using different gamma ray sources such as ^{137}Cs and ^{60}Co. The results showed that the above-mentioned material is a promising and a potential candidate for scintillation and neutron detection applications.

e0004

***In vitro* bioactivity of bismuth containing borate-based glasses**

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Bismuth containing borate-basedglasses wereprepared by conventional melt-quenching technique and characterised to know their biological activity suitable for tissue engineering applications. Bioactivity of glass samples was examined*in vitro* by the apatite mineralization ability in simulated body fluid (SBF). The glass samples were analysed by XRD, FTIR and SEM-EDS before and after immersion in SBF. The obtained results revealed that the developed bismuth containing borate-based glasses have shown excellent hydroxyapatite layer (HAP) formation in SBF for lower content of bismuth. Therefore, the prepared bismuth borate glasses are appropriate for the development of bioactive implants.

e0005

γ-ray Induced Defects in Yb^{3+}-Sm^{3+} Co-doped Borate Glass

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The $10BaO\text{-}20ZnO\text{-}20LiF\text{-}49.4B_2O_3\text{-}0.1Yb_2O_3\text{-}0.5Sm_2O_3$ glass was studied for the structural and optical changes after 1 kGy γ-dose exposure. Post-irradiation, the Fourier Transform Infrared spectroscopy indicated the upsurge in Non-Bridging Oxygens while the optical absorption spectroscopy revealed the occurrence of color centers and rise in defects. The defect centers were distinguished as Non-Bridging Oxygen Hole Center and Boron *E'*-center from the Electron Spin Resonance analysis.

e0006

Dielectric and AC Conductivity Studies of CdZnTe Quantum Dots Doped Silica Matrices

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CdZnTequantum dot doped silica matrices synthesised through sol-gel route using acid catalyst. The prepared silica matrices with different concentrations of CdZnTe quantum dots were characterized using FTIR and EDX spectrum. The effect of CdZnTe nanocrystals doping on the dielectric properties of sol-gel silica glasses was studied for a frequency range of 100 Hz- 5 MHz at room temperature. The frequency dependence of dielectric constant real part, loss tangent and A.C conductivity were investigated. The conductivity curve obeys Jonscher's power law and power law parameters were found out.

e0007

Effect Of Te Content On The Optical, Structural And Morphological Properties Of $Ag_{(60-x)}Se_{40}Te_x$ Thin Films

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The present work investigated the effect of tellurium concentration on structural, optical, and morphological properties of the $Ag_{60-x}Se_{40}Te_x$(x=0,5,10 at %) thin films. The studied thin films were prepared by the thermal evaporation method from bulk sample. The XRD study showed no change in the amorphous behavior withthe increase in Te concentration and the corresponding changes in the vibrational level have been studied from the Raman analysis. The change in the surface morphology with Te concentrationhas been observed fromAFM and FESEM pictures, while the compositional analysis has been done by EDX. The UV-Vis spectroscopy study revealed that an increase in the dopant concentrationenhances the transmittance, whereasreduces the optical bandgap of the material. This reduction in the bandgap was explained by takingthe chemical bond approach, where the increase in Te content reduces the cohesive energy that led to the reduction of the bandgap.

e0008

Effect Of Modifier On Spectroscopic Properties Of Lead Bismuth Phosphate Glass System Mixed With Neodymium (III) Oxide

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PbO─P2O5─ Bi2O3─R2O3 (R = Al, Ga, In, Tl) glasses doped with Nd2O3 were prepared by melt quenching technique. The prepared glasses were characterized by the XRD patterns. Conventional spectroscopic studies viz., optical absorption, photoluminescence studies were carried out on these glasses. The optical absorption spectra exhibited eleven absorption bands around 351,431,473,514,526,581,628,683,747,804 and 874 nm wavelength corresponding to the transitions 4I9/2 →4D1/2, 2P1/2, 2G9/2, 4G9/2, 4G7/2, 4G5/2, 2H11/2, 4F9/2 , 4F7/2, 4F5/2 and 4F3/2 respectively. Judd-Ofelt(J-O)parameters have been evaluated for the prepared glasses using optical absorption spectra and these J-O intensity parameters have exhibited the trend Ω2> Ω6 > Ω4. Emission spectra of the prepared glasses were recorded at the excited wavelength804nm and it exhibited three prominent peaks at about 885, 1054,

1323 nm wavelength corresponding to the 4F3/2→4I9/2, 4I 11/2, 4I13/2 transitions levels respectively in the near infrared region. By using the J-O parameters various radiative parameters for the excited luminescent levels of Nd3+ ions are evaluated. Emission cross section and branching ratio values are observed to be high for4I11/2 level of Nd3+ ions The above investigations indicate that the glass system mixed with Ga2O3 could be a suitable candidate for 1.06 μm laser source in the near IR region

e0009

Structural and Nuclear Radiation Shielding Properties of Barium-Sodium-Alumina-Borate Glass System

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In the present study, physical and structural parameters of Barium-Sodium-Alumina-Borate glass system such as density, molar volume, oxygen packing density (OPD), oxygen molar volume (OMV), ion Concentration, Polaron radius, inter-ionic distance and field strength have been calculated. The elastic parameters namely Young, bulk, shear moduli, and Poisson's ratio of the glass samples have also been calculated using the Makishima and Meckenzie model. Further, in order to study the application of selected glass system in the field of nuclear radiation shielding and design, the values of attenuation parameters and fast neutron removal cross-section ($\sum R$ cm^{-1}) were calculated and compared with standard radiation shielding materials.

e0011

Structural Studies Of Silver Doped Lithium Bismuth Borate Glasses

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Silver oxide doped lithium bismuth borate glasses have been prepared by the conventional melt quenching method with compositional range $30LiF\text{-}40Bi_2O_3\text{-}(30\text{-}x)B_2O_3\text{-}xAgNO_3$(x=0,0.1,0.5 and 1 mol%).Structural studies were characterized using FTIR spectroscopy. The density of glasses were determined. The incorporation of silver causes some structural rearrangement in the glass network leads to formation of BO_4 and BO_3 structural units. BO_4 are the dominant structures formed in this glass network.It is observed that with progressive silver doping there is appearance and disappearance of some IR bands in the BO_4 spectral region. Silver acts as network modifier as it promotes the conversion of four coordinated to three coordinated boron initially and reversed afterwards.

e0012

A frequency-dependent dielectric study on the amorphous biopolymer electrolyte membrane

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The present work studies the dielectric properties of NaSCN incorporated sodium alginate-based amorphous biopolymer electrolyte membranes. From the impedance measurements, frequency-dependent real and imaginary parts of the dielectric permittivity and electric modulus have been calculated. The dielectric permittivity of the electrolyte membrane is high at the low-frequency region which validates the electrode-electrolyte polarization. The

electric modulus for the salt-concentrated membranes gets decreased with respect to frequency. The investigation divulges the frequency-dependent behavior of the ions in the sodium alginate biopolymer system.

e0014

Study Of Optical Constants Of $Ge_{25}S_{75-x}Sb_x$(x=0, 10, 20) Amorphous Chalcogenides For Optical Applications

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Amorphous $Ge_{25}S_{75-x}Sb_x$(x=0,10,20) chalcogenides are processed by familiar melt quenching approach and vacuum thermal evaporation approach for preparing alloys and then thin films respectively. An optical transmission experiments have been done in the given samples. Swanepoel method has been used to calculate various optical parameters. Tauc's relation has been used for the estimation of optical band gap. An indirect optical transition has been found for present glassy system and on the basis of optical parameters the suitability has been discussed for various optical applications.

e0015

Structural and Optical analysis of Cadmium Bismuth Borate glass system

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Cadmium doped sodium bismuth borate glasses have been synthesized by melt quenching technique. Physical, optical and structural properties have been explored by UV-Vis spectroscopy, X-ray diffraction (XRD) and Fourier Transform Infrared spectroscopy (FTIR). Interesting results are observed; thereby confirm the change in structure of the host glass with addition of Cadmium.

e0016

Structure determination of Lead Iron Phosphate Glasses

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Reverse Monte Carlo modelling of total neutron diffraction data of Lead Iron Phosphate glasses have been performed to determine the structural origin of high leaching resistance behaviour shown in these glasses. Effect of Fe_2O_3 concentration on the atomic structure and its correlation on leaching resistance is probed.

e0018

Glass transition temperature dependence on coordination number for quaternary Se-Te-Ge-Pb alloys

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In the present work, differential scanning calorimetry (DSC) is employed for thermal study of $(Se_{80}Te_{20})_{94-x}Ge_6Pb_x$($x$=0, 1, 2, 4, 6, 8, 10 and 12) bulk samples under non-isothermal conditions. Glass transition temperature (T_g) of investigated alloys has been deduced theoretically using Tanaka approach and modified Gibbs DiMarzio relation. Dependence of T_g on average coordination number (<r>) is analyzed. Trends of experimental and theoretical results are not in agreement with each other which show T_g does not solely depend on <r>.

e0020

Synthesis and Characterization of Semiconducting Iron Tellurite Glasses

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xFe_2O_3-(100-x)TeO_2 (where x = 15 and 30 mol%)glasses were prepared by normal quenching technique. The samples were characterized by X-ray diffraction, DSC, Raman spectroscopy and dc electrical conductivity studies. The density of glasses decreases from 5.34 to 5.14 gcm^{-3} and glass transition temperature increases from 659 to 710 K as the concentration of Fe_2O_3 is increased from 15 to 30 mol%. Raman studies reveal that the Te-O coordination number decreases from 3.55 to 3.48 while the room temperature electrical conductivity increases from 1.79×10^{-7} to 4.00×10^{-5} $\Omega^{-1}m^{-1}$ with an increase in concentration of Fe_2O_3 from 15 to 30 mol%.

e0024

XAFS Characterization Of Self-irradiated Gadolinite

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Immobilization of radioactive wastes in suitable hosts is pressing industrial demand. We have conducted XAFS investigation for (Fe, Y)-site resolved structure and valence information in such a potential host - Karatupatti metamict gadolinite ($FeO_{10}Be_2Y_2Si_2$) from (South India).We detected multi-site configuration that drives large disorder of Fe(Y)-O-Si linkage. Implications of large disorder for actinide immobilization and its thermal recovery are discussed.

e0025

Structure property relations in $(As_2Se_3)_x(GeTe_4)_{100-x}$glasses

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$(As_2Se_3)_x(GeTe_4)_{100-x}$ glasses were prepared over the entire composition range $0 \le x \le 100$. As_2Se_3 is an excellent glass former and its increase is expected to improve the glass forming ability (GFA) of $(As_2Se_3)_x(GeTe_4)_{100-x}$. In contrast, GFA shows an opposite trend. Initial addition of As_2Se_3 ($x < 40$) depolymerises the network and affects the glass forming ability. Glass transition (T_g) shows a decreasing trend for $x < 40$ and the network is mainly dominated by Ge-Te units. For $40 \le x \le 60$, the network is modified from Ge-Te to As-Te based units. The structural network also begins to polymerize but the average bond energy becomes low. In this range, T_g is found to remain unchanged as both network connectivity and average bond energy compete with each other. For $x > 60$, T_g is found to increase as both the average

bond energy and the network connectivity are increasing. From the Raman studies, the presence of $GeTe_{(4/2)}$, $GeSe_{(4/2)}$, Te-Te, $AsTe_{(3/2)}$, Se-Te and $AsSe_{(3/2)}$ structural units are inferred. The glassy network is dominated mainly by $GeTe_{(4/2)}$ for $x < 40$, and for $x > 60$, the network is dominated by $AsSe_{(3/2)}$ structures. Glasses in the intermediate compositions $40 \leq x \leq 60$ are composed of mixed structures $GeSe_{(4/2-k/2)}Te_{(k/2)}$, Te-Te and $AsTe_{(3/2-n/2)}Se_{(n/2)}$. These results bring out the dominance of chemical composition effects over the network connectivity in a critically coordinated network.

e0027

Elastic constants for the inhomogeneous amorphous states of the hard sphere system

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We study the high frequency elastic constants for the metastable amorphous states of the hard sphere liquid. The disordered states are identified using the classical density functional theory(DFT) model modified to consider the highly inhomogeneous states. We observe a cross in the behavior of the DFT elastic constants for the two qualitatively different types of amorphous states signifying different degrees of mass localization in the system. We also obtain the high-frequency elastic constants for the homogeneous state using the well-known Mountain-Zwangig formula.

e0028

Replica Theory For Structural Glass Transition Using Density Functional Hamiltonian

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We study microscopic replica field theory of the disordered system without quenched disorder. The sharp fall of configurational entropy of a many-particle system is analyzed with the scenario of spontaneous ergodicity breaking, in which the free energy landscape of the many-particle system splits into distinct basins of local minima. The field theoretic model is formulated in terms of a density field, and a nonlocal free energy functional used in classical density functional theory (DFT) up to third order in density fluctuation $\delta\rho$ is the key input in the calculation. Using a mapping into a composite system of m replicas, and idea of an an auxiliary field, first suggested by R. Monasson, We compute the configurational entropy S_c of the supercooled liquid. The configurational entropy S_c sharply falls with increase of packing fraction η_k.The Kauzmann point η_k is obtained in the model is in agreement with other works.

e0029

Bi_2O_3 Glasses: Gamma Ray Shielding Properties

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Quaternary glass systems containing oxides of bismuth based glass systems: S1 ($3Bi_2O_3$-$62B_2O_3$-$15Li_2O$-$15K_2O$-$5MoO_3$), S2 ($3Bi_2O_3$-$62B_2O_3$-$15Li_2O$-$15K_2O$-$5V_2O_5$ and S3 ($0.65Bi_2O_3$-$0.15B_2O_3$-$0.15Na_2O$-$0.05BaO$) have been prepared by melt quenching technique using AR grade chemicals. Gamma ray shielding parameters in terms of mass attenuation coefficient, HVL and MFP have been calculated at photon energies 356, 662, 1173 and 1332 keV. Prepared samples provide better radiation shielding properties than some standard concretes.

e0030

Effect of Neodymium Loading in Iron Phosphate Glass

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A series of iron phosphate glass (IPG) samples loaded with different mole percent of Neodymium (Nd) oxide were prepared by melt quench technique with a view to test the feasibility of high-level waste immobilization in them since Nd is considered to be a chemical surrogate for actinides like Curium (Cm). Typically, for a batch of 25g, the constituent oxides in stoichiometric ratio are melted at a temperature of 1323K, quenched in air and vitrified on a steel plate. Scanning electron micrographs of representative samples showed that they were homogeneous in terms of composition, devoid of any noticeable precipitation of crystalline phase and nodule formation up to 8mol%. The observation was further confirmed from the overlapping EDS elemental mapping of the samples. Amorphous nature of the samples was ascertained from their respective X-ray diffraction patterns which showed broad hump in between 20^{o}-30^{o}. Thermogravimetric analysis of the samples confirmed their stability over a wide range of temperatures, which was further substantiated from their glass transition temperatures (T_g), liquidus temperature (T_L) and crystallization temperature (T_x) obtained through the calculation of K_H, K_W and K_{LL} parameters. It was observed that the IPG matrix got structurally modified upon incorporation of Nd.

e0031

Gamma Attenuation by Cadmium Chloride filled Polymeric Blend Composite at Specific Gamma Photon Energies – A Computational Approach

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The mass attenuation coefficient and half value layer thickness of composite films comprising polyvinyl alcohol – polyvinyl pyrrolidone blend reinforced with cadmium chloride has been explored by a computational method at specific gamma photon energies, equal to 14.4, 31, 59.54, 80, 122, 356, 511, 662, 835, 1173, 1274 and 1332 keV. Data from NIST- XCOM has been used to extract the necessary basic information in order to perform the computations. The FLs of cadmium chloride in the polymeric blend considered for the computational study are 5.4, 10.2, 15.5, 21.5, 30 and 40 Wt%, which were selected based on the composites prepared for earlier microstructural studies on this system. The half value layer thickness decreases on the increased incorporation of filler into the host polymeric blend, at all the gamma photon energies of interest, implying that the material can be effectively used as a gamma shielding material.

e0032

Nano Silver (Ag^{+}) Ion-Exchange Composite Glass for Enhanced Linear and Nonlinear Optical Properties

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Silver nanocomposite (Ag-NCs) glasses are formed by sequential ion-exchange and thermal annealing technique.The dielectric containing the metal nanoclusters are well investigated by optical absorption (OA) showed the signatures of Ag^{+} clusters embedded in the glass-matrixexhibiting OA peak due to dipolar Surface Plasmon Resonance (SPR). Low frequency Raman Scattering (LFRS), which stemsfrom the quadrupolar acoustic vibrations of the embedded Ag-nanoclusters and PL band centered at 445 nm.Open aperture *z*-scan measurement shows the transmitted light was recorded as a function of the sampleposition along the focal plane. The spectrum was fitted using the theory and the magnitude of the nonlinear absorption coefficient was determined from it.

e0033

Different Models For Calculating The Refractive Index And Band Gap For Chalcogenide Glasses

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Optical analysis plays an important role in the development of optoelectronic materials. In this paper, some relations have been studied for optical parameters for erbium based GeSbSe system. These relations are based on the particular models suggested for calculating doped, co-doped *etc.* chalcogenide systems for a given energy gap range. These models predict refractive index values and are compared to the experimental analysis of chalcogenide glasses. The experimental refractive index for $Ge_{17}Sb_8Se_{75-x}Er_x$ (x=0, 0.4 and 0.8) thin films varies from 2.45 to 2.67 and have good agreement with the relationships proposed by several researchers.

f: SURFACES, INTERFACES, AND THIN FILMS

f0002

Spin-Coated ZnO Nanocrystalline Thin Films: Effects Of (Sn, Ni) Co-Doping On Their Microstructural And Optical Properties

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In this paper, the effects of (Sn, Ni) co-doping on the microstructural and optical properties of the spin-coated ZnO thin films have been investigated. The crystallinity of the films has been found to be maximum in the undoped ZnO film with preferred orientation along (0 0 2) plane. Upon doping and co-doping, the film crystallinity decreases. The energy band gap value of the undoped ZnO film is found to be 3.26 eV, which decreases slightly upon doping and co-doping. The refractive index values of the doped and co-doped ZnO films are found to be more than that of undoped ZnO film.

f0003

Evaluation of Optical Parameters of ZnSe Thin Film

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Zinc Selenide (ZnSe) thin film was fabricated onto an ultrasonically clean glass substrate by physical vapour deposition method under high vacuum. The value of optical band gap was found to be 2.62 eV evaluated using absorption spectra. The low value of Urbach energy and the interference pattern in absorption spectra the film has a good surface smoothness, low defects and is uniformly deposited onto glass substrate. Also, the position of conduction band and valence band of ZnSe thin film was calculated using semi-empirical relation.

f0004

Induction Time Induced Modifications in Physical Properties of Chemically Grown nanorystalline PbS Thin Films

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Nanocrystalline lead sulfide (PbS) films are prepared on glass substrate by using simple, low cost chemical bath deposition (CBD) technique by varying the induction time. The induction time induced effects on physical properties are studied with the help of X-ray diffraction pattern (XRD), Raman spectroscopy and UV-Vis spectroscopy. From the XRD patterns, it can be seen that the as the induction time of thin films increased the nature of appearance turned into polycrystalline in nature with cubic phase, while the average crystallite size observed to be ~22nm. Raman spectrum analysis confirms that CBD method suits best for synthesis of stiochiometry nanocrystalline PbS thin films. The electronic transitions studied using the optical absorbance spectra shows that the absorbance coefficient increases with increase in induction time.

f0005

Proton Ion Irradiation Induced Changes In Optical And Morphological Properties Of $As_{40}Se_{50}Sb_{10}$ Thin Films

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The impact of proton irradiation (30 KeV) upon the optical and morphological properties of thermally evaporated $As_{40}Se_{50}Sb_{10}$ thin films was observed in our study. The transmittance and RMS roughness of the irradiated films significantly increased with higher fluence. The optical bandgap and refractive index changed with fluence. The tuning of different optical parameters and surface modifications with proton ion fluence are suitable for optical applications.

f0006

Bovine Serum Albumin/Lysozyme (BSA/Lys) Complex Thin Film

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The protein complex formed by mixing two globular proteins, bovine serum albumin (BSA) and lysozyme (Lys), is studied using Langmuir-Blodgett method. The surface pressure (π)-specific molecular area (A) isotherm of the monolayer formed at the air-water interface at a subphase pH $\approx$ 9.0 shows a rise in surface pressure at $A \approx 52$ nm^2/molecule and a plateau-like feature is observed at $\pi \approx 18$ mN/m. Atomic force microscopy (AFM) gives an average height of 1.26 nm and a total height of 4.28 nm, whereas x-ray reflectivity analysis gives a thickness of $\approx$ 41Å of the deposited complex film in single up-stroke. Thus a stable protein complex film can be formed at the air-water interface which may have potential applications.

f0010

Influence Of The Substrate Temperature On The Structural, Optical, And Morphological Properties Of (101) Oriented ZnSe Thin Films For Solar Window Applications,

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Structural, optical, and morphological studies of spray deposited zinc selenide (ZnSe) thin films at various substrate temperatures are reported. Films were characterized using energy dispersive analysis (EDX), x-ray diffractogram (XRD), and UV-Vis spectra. ZnSe thin films showed a strong preferred (101) orientation with an excellent crystallite size of 57.4 nm at a deposition temperature of 673 K. Composition of Se/Zn was 0.8. A transmittance of nearly 75% was observed in the visible regime, with a wide band gap of 2.7 eV; the prepared samples were assessed for window layer in solar cells.

f0011

Effect of Oxygen Annealing on Ultrafast Carrier Dynamics of $Pr_{0.5}Ca_{0.5}MnO_3$ Thin Films

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We report the effect of oxygen annealing and epitaxial strain on the ultrafast carrier excitation and relaxation mechanism of hole-doped manganite $Pr_{0.5}Ca_{0.5}MnO_3$ (PCMO) as investigated by optical pump-Terahertz (THz) probe measurements. PCMO thin films of 60 nm thickness, both pristine and oxygen annealed, were prepared using pulsed laser deposition technique. Transient THz transmittance is negative for both the films. As fitted by the sum of exponentials, the fast relaxation time constant is found to be fluence independent while the slow relaxation time constant decreases with pump fluence for both the films and is less for the annealed film suggesting that the relaxation in PCMO strongly depends on strain and oxygen content.

f0012

Structural and Magnetic Properties of Bi_2FeReO_6 Double Perovskite Thin Films

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Ferromagnetic insulators (FMI) are the most promising candidates for the application in the field of dissipation less electronics as well as spintronics. Devices operating at practical conditions are highly desirable. In this context, we have examined the effect of epitaxial strains on magnetism of Bi_2FeReO_6 (BFRO) thin films prepared by the pulsed laser deposition technique. The effects of crystallographic orientations on structural and magnetic properties were investigated. Our studies reveal that the magnetization of these thin films is strongly dependent on tensile and compressive strains as well as on crystallographic orientation along strain is induced.

f0013

Optimization of Spray deposited Ca-Doped SnO_2 thin films for Ethanol Gas Sensor Application

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The Ca-doped SnO_2 (CTO) thin films are spray deposited on glass substrate as a function of solution concentration for the ethanol gas sensor Applications. The X-ray diffraction pattern of the film deposited from 0.2 M, 0.5 M, and 1.0 M solution concentration possesses the SnO_2 phase with a tetragonal crystal structure. The surface morphology of the spray deposited thin films confirms nanoparticle formation with the lower surface roughness. The ethanol gas fabricated using a 0.5 M solution (CTO-2) exhibits the maximum sensitivity of 69.7 % with a response and recovery time of 114/98 s. Hence, the optioned results confirm the applicability of CTO thin film as an ethanol gas sensor.

f0014

In-situ RHEED study of reactively sputtered ScN thin films

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We report a nascent real time structural analysis of reactively sputtered ScN thin films through in-situ RHEED. Samples were grown on single crystalline MgO (001) substrates at different substrate temperatures (T_s). Notably, at room temperature, the adatom mobility was insufficient leading to a polycrystalline growth. However, increasing the T_s to 523 and 773 K enhances the crystalline growth and self-sustaining the epitaxial nature along the [100] azimuth up to a comparatively high thickness. However, at T_s = 973 K, resulting films again show the polycrystalline growth due to N out-diffusion leading to a N-deficient Sc-N phase .

f0017

Oxygen Pressure Dependence Of The Growth of $La_{0.66}Sr_{0.34}MnO_3$ Thin Films And Their Magnetic Anomalies

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We have setup a ultra-high vacuum pulsed laser deposition system and have grown $La_{0.66}Sr_{0.34}MnO_3$ films on $SrTiO_3$ (001) substrate under different oxygen partial pressures. The samples show good crystallinity and mosaicity. The lattice parameter of the films decreases with the increase in oxygen pressure. Curie temperature, T_C of the deposited films are found to be below the room temperature which is much lower than the reported values for both bulk and thin film samples. Interestingly, *M-H* isotherm at 300 K shows clear hysteresis. Such anomalous behavior indicates the presence of some magnetic order even above T_C of this system.

f0018

Impact of Post MgI_2 Treatment on Properties of CdS Films for Solar Cells

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The polycrystalline pristine thin films consist of large amount of grain boundaries which are detrimental for devices and need passivation by $CdCl_2$ chloride treatment. The toxic nature of $CdCl_2$ emphasizes to expose its alternative compounds, and therefore in this study, an impact of post deposition MgI_2 (Magnesium iodide) treatment on the structural, optical and electrical properties of thermally evaporated CdS thin films is undertaken. XRD patterns reveal that the CdS thin films consist of hexagonal phase with (110) preferred orientation where the crystallite size is observed in range of 37-48 nm. The electrical analysis showed the linear change in current with voltage with decreased conductivity. Optical study demonstrated that direct optical energy bandgap of MgI_2 passivated CdS films is increased from 2.2 to 2.5 eV with temperature. Thus, MgI_2 treatment has influenced the properties of CdS films at a great deal, and consequently, CdS thin films annealed at 200°C are found appropriate for window layer in Cd-based thin film solar cells.

f0019

Annealing Induced Properties of ZnTe:Cu Back Contact Layer for Solar Cells

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In order to realize the entire potential to the CdTe thin film solar cells, the development of environmentally stable, low-resistive, and easily manufactured back contact is required. The Cu doped zinc telluride i.e. ZnTe:Cu interface layer is most suitable for back contact applications between the CdTe and the metal contact. The annealing is proved to be an effective way for improving the properties of films. Therefore, the present work demonstrates the physical properties of ZnTe:Cu 5% films where films are deposited thermal evaporation technique and annealed in air ambient in 100-300°C temperature range. The developed films showed (103) preferred orientation where the crystallite size is found in the range of 38-44 nm. The transmittance of ZnTe:Cu 5% films is varied with temperature and optical energy band gap is estimated in the range of 2.71-2.80 eV. The electrical analysis of ZnTe:Cu 5% films confirmed their ohmic behavior.

f0021

A Sensitive NH_3 Sensor Using $MoSe_2/SnO_2$ Composite

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In this report, we demonstrate the use of p-$MoSe_2$/n-SnO_2 heterojunctions as sensitive and selective chemiresistive ammonia sensor operating at room temperature. The $MoSe_2/SnO_2$ composite was synthesized via a two-step synthesis approach. Structural analysis was confirmed by Raman spectroscopy. Two-terminal devices were made on an alumina substrate with pre-deposited gold contacts. The resulting composite device showed n-type semiconductor behavior. Surprisingly, the composite based sensing device exhibited enhancement in ammonia sensing as compared to $MoSe_2$ (p-type) and SnO_2 (n-type) counterparts. The device also displayed excellent response and recovery features together with a superior selective nature towards ammonia as compared to ethanol, acetone, and formaldehyde. The current study demonstrates the potential application of composite-based heterostructures for NH_3 detectiion.

f0022

Effect of Pyrochlore phase on Magnetic Properties of PMN-PT/LSMO Thin film

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In this paper, we demonstrate the effect of the pyrochlore phase on magnetic properties of $La_{0.30}Sr_{0.70}MnO_3$ in PMN-PT/LSMO bilayer thin film grown on (001) oriented LAO single crystal substrate using pulsed laser deposition technique. The formation of the pyrochlore phase at 34^0 in thin-film probed using X-ray diffraction θ-2θ scan. There is a reduction in M_S value and enhancement of T_C occur in PMN-PT/LSMO/LAO thin film compared with LSMO/LAO. The pyrochlore phase relaxes the strain and induces oxygen deficiency in both the PMN-PT layer and PMN-PT/LSMO interface, which restore the Mn-O-Mn bonding and create an imbalance in Mn^{3+}/Mn^{4+} valance ratio, thus reducing the magnetization value of LSMO. The compressive strain of LSMO in PMN-PT/LSMO/LAO (ε_{out}=1.03%) thin film is less than LSMO/LAO (ε_{out}=1.28%), which might be shift the T_C of bilayer thin film towards bulk value ($365\ ^0$C).

f0023

Electrochemical impedance spectroscopy study of protective aluminium thin film coatings on AZ31 Mg alloy against corrosion

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Magnesium is the lightest structural element that struggles for its proper application because it is highly corrosive under wet environment. A good protective surface coating on it would help to improve its corrosion inhibition capability. In this direction, aluminium metal coating on the Mg alloy AZ31 is chosen in this work. Thermal evaporation technique was employed to achieve aluminium coating of varying thicknesses in the range from 50 nm to 200 nm. Scanning electron microscopy studies showed a uniform Al coating on the AZ31 substrate. Electrochemical impedance spectroscopy technique was used to study the corrosion behaviour of the coatings. The coatings were exposed to corrosive environment for 12 h and their performance was evaluated.

f0024

Blue shifted photoluminescence emission of ion beam modified InGaP thin film

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In this report we have studied the photoluminescence (PL) property of the ion beam modified InGaP ternary thin film grown on GaAs substrate. The sample is irradiated with 200 keV N^+ ions and subsequently ion beam annealed with 2 MeV He^+ ions. The pristine InGaP sample exhibits PL emission in the near IR region centered around 670 nm, whereas, the irradiated sample exhibits PL emission in the visible region centered around 520 nm. The Rutherford backscattering spectrometric analysis of the samples evidenced that there is no significant change in the composition or thickness of the film upon ion irradiation. Thus our studies have shown that ion irradiation can alter the local electronic structural property of the ternary film which results a large blue shift in the PL emission.

f0025

Characterization of Interface of Corn-Husk Film Reinforced Composites

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There is abundance of lignocellulose-based biomass globally, but the most challenging task is to increase the quality of the interface between reinforcement and matrix in order to achieve desired properties from the selected combination of filler and matrix as a whole. In present research interface between corn-husk film (CHF) and epoxy matrix is characterized through SEM, XRD, FTIR and dynamic mechanical analysis (DMA). SEM micrographs of fractured samples of treated CHF show better interphase between CHF and epoxy as compared to untreated CHF. Alkali treatment enhances the fibre surface texture and reduces impurities on the external surface of the fiber which resulted in improved interface and as well as mechanical interlocking between matrix and reinforcement. Dynamic properties improve with addition of CHF in the composites and the best results are obtained at 6wt % CHF and 45^0 angle of orientation of CHF. The improved interface between CHF and epoxy matrix widens its scope for applications in automobile and construction sector.

f0026

Effect of Annealing on the Physical Properties of Absorber $Cd_{0.95}Zn_{0.05}Te$ Thin Films for Solar Cells

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Annealing plays a crucial role in modifying the physical properties of thin films, hence, the present work deals with the effect of annealing on the physical properties of 800 nm thin $Cd_{0.95}Zn_{0.05}Te$ films deposited employing thermal evaporation technique. Structural analysis revealed that the pristine and annealed films are inclined towards (220) cubic plane and crystallite/grain size increased with annealing. The electrical analysis demonstrated the ohmic nature of the pristine and annealed films with decreasing conductivity. The optical analysis depicted variation in the optical absorbance where the band gap of the pristine and annealed films is found in the range 1.70-2.76 eV. The attained results indicate that the films annealed at 300°C are apt as absorber layer for the fabrication of high efficiency single junction and tandem solar cell devices concerned.

f0027

Spectroscopic Analysis of PVD Deposited Indium Selenide (In_2Se_3) Thin Films for Photodetector Applications

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The manuscript presents spectroscopic studies of the Indium Selenide (In_2Se_3) films, which are grown via thermal evaporation technique. The deposited films are amorphous in nature and uniform throughout the substrate as confirmed by SEM/EDS results. The transmittance and absorbance spectrum were taken by spectrophotometer, and direct band gap was found to be 1.95 eV. The vibration mode was studied by Raman spectra and PL emission occurs in the UV and near IR region. The spectral response of the deposited films was high for 635 nm wavelength and suitable for visible range photodetector applications.

f0028

Structural Characterization of Thermally Annealed ZnO Thin Film Grown on Si (111) by RF Sputtering

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This work presents the effect of thermal annealing on the structural properties ZnO thin film deposited on p-type Si (111) substrate using radio frequency sputtering technique. GIXRD pattern reveals the formation of polycrystalline ZnO thin film having hexagonal wurtzite structure with preferential growth along (002) plane. After annealing at 800°C, it has been observed that intensity of peak corresponding to another orientation i.e. (103) increases pointing towards the modification of surface chemistry due to heat treatment. Further increase in temperature to 900°C enhances the crystallinity of ZnO thin films. The hexagonal wurtzite structure of films is confirmed using FESEM.

f0029

Formation of a crystalline and magnetic alloy phase (Fe_3Ge) at the interfaces of Fe/Ge multilayers

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@This paper is dedicated to the memory of Dr. C. L. Prajapat, who passed away on 10th September 2021

Ferromagnet-semiconductor (FM-SC) alloy phase with room temperature ferromagnetic properties at the interfaces of FM/SC heterostructures are believed to improve the electron spin injection from the FM to the SC for the realization of spintronic devices. Here we report the formation of a crystalline alloy phase (Fe_3Ge) at the interfaces on growing ultrathin Fe/Ge multilayers at an elevated substrate temperature of ~ 523 K as well as on annealing the multilayer at a temperature > 523 K. The alloy phase formation at interfaces is achieved at a much lower temperature than the Fe_3Ge phase formation in bulk material (~ 973 K), mainly due to rapid interdiffusion of Fe and Ge at the interfaces**.**

f0030

Design of Non-periodic and periodic multilayer for high energy X-ray application and optimization of process parameters

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Systematic arrangement of non-periodic multilayer can reflect a band of high energy X-ray and periodic multilayer of ultra-low bi-layer thickness can divert particular energy of X-ray in grazing angle geometry. Non-periodic W/Si multilayer has been designed for X-ray telescope application to cover up to 69.5 keV energy and WC/SiC periodic multilayer has been designed to divert 100 keV energy for direct measurement of U and Pu in spent fuel. The multilayer for X-ray telescope has been designed in two techniques and compared. In order to fabricate WC/SiC multilayer deposition power of in-house developed DC magnetron system has been optimized and a periodic multilayer of 10 bilayer has been fabricated

f0031

Structure and Growth Mechanism of Thin Film of DNTT Molecules on SiO_2/Si Substrate

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The structure, molecular orientation, and surface morphology of the dinaphtho[2,3-b:20,30-f]thieno[3,2-b]thiophene (DNTT) molecules on SiO2/Si substrate, deposited by thermal evaporation, were investigated using X-ray reflectivity (XR) and atomic force microscopic (AFM) techniques to understand the growth mechanism of the thin film on dielectric SiO2 surface, which has a strong influence on the charge transport properties of the DNTT based devices. The upright molecular orientation of the DNTT molecules and their crystallinity in thin film were realized by analyzing the XR profile and XRD maps in specular and off-specular directions, while the closely spaced domain-like structure of the DNTT thin film with high surface roughness was evident from AFM images.

f0032

Room Temperature Gas Sensing Properties of H-terminated Diamond

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Hydrogen termination on diamond surface (HD) makes the surface conductivity to be very high with p-type doping through water adlayer mediated electrochemical charge transfer process. When the HD surface is exposed to chemical gases which undergo electrolytic dissociation, the surface conductivity changes greatly due to the disruption of charge equilibrium at the diamond/adlayer interface and this offers advantages for selectivity in gas sensor applications. Here, we report on the gas sensor response of HD towards H_2S at room temperature in ambient air. The HD sensor device exhibits a linear response from 5 to 70% for H_2S in the concentration range of 10 to 90 ppm in ambient air. The gas sensing mechanism of HD is discussed in brief.

f0033

Amorphous Hydrogenated Germanium as Passivation coating on High Purity Germanium Detector: Optimization of film parameters

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Amorphous hydrogenated germanium (a-H-Ge) has emerged as a suitable passivant for HPGe detectors. The properties of the a-H-Ge affect the performance of the resultant detectors, and these properties substantially depend on and are controllable through the sputter deposition process parameters. The subject of this paper is this interconnection of fabrication process parameters, a-Ge film properties, and detector performance. Films deposited at high sputter pressure show high resistance and are capable of inhibiting surface leakage current of the fabricated HPGe detector considerably.

f0034

Ag_2O Decorated ZnO Nanorods Demonstrating Two-Step Visible-Light Photocatalytic Dye-Degradation Phenomena

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ZnO/Ag_2O heterostructures, as the functional materials for photodegradation of MB dye under visible light irradiation, have been achieved using inexpensive hydrothermal and ultrasonic-assisted synthetic routes. The heterostructures had wurtzite ZnO peaks that were highly crystalline and hexagonal, as well as cubic Ag_2O peaks. The ZnO/Ag_2O photocatalyst demonstrated two dye degradation slopes, with the higher-slope arising later in the process, when metallic-Ag traps the valence electrons of Ag_2O nanoparticles and advances e^-/h^+ separation across ZnO/Ag^0/Ag_2O heterojunction structures, making them readily accessible for superior dye degradation.

f0035

Diamond-Like Carbon Thin Films from Low-Pressure and High-Density CH_4 Plasma

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DLC thin films were grown using a low-pressure high density CH_4/Ar plasma on glass substrates in a planar RF (13.56 MHz) Inductively Coupled Plasma CVD system. Using a plasma triggered by RF power to a mixture of 20 sccm CH_4 and 50 sccm Ar gas maintained at a low pressure of ~30 mTorr, a series of samples were prepared by varying the substrate temperature and then changing the RF power. The optimised DLC films, obtained at 500 °C and 900 W demonstrated high optical transmission of ~97 %, wide optical band gap of ~3.58 eV and a minimum of I_D/I_G ~0.61 and a maximum of I_{Dia}/I_D ~1.32 in Raman analysis demonstrated the maximum sp^3/sp^2 content in the carbon network.

f0036
Probing Carrier Traps by Photocurrent Transients in Sputtered ZnO Thin Films Grown Without and With O_2
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ZnO films have been deposited under various Ar and O_2 gas flow by RF sputtering method. The photoluminescence measurements suggest a decrease in the radiative defect levels. Huge decrease in the dark current and therefore highly enhanced ultraviolet photosensitivity with an increase in the O_2 flow during growth indicates a decrease in the donor defects. The photocurrent transient spectroscopy indicates majority carrier traps mainly lie within 2.06 eV for the film deposited with only Ar whereas within 2.06 to 2.48 eV below the conduction band for the films deposited with Ar and O_2.

f0037
Effect of H_2-Dilution for Growing nc-SiGe Thin Films in PECVD
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Hydrogen dilution facilitates for sustaining nanocrystallinity in SiGe thin films, simultaneously minimizing the difference in the decomposition rate of two source gases GeH_4 and SiH_4 in the plasma. At a H_2 dilution ratio $R(H_2)= [H_2]/[(SiH_4)+(GeH_4)] = 50$, nc-SiGe thin film with high crystallinity possessing dark conductivity σ_D ~1.54×10^{-2} S cm^{-1} and optical band gap, E_g ~ 1.55 eV has been prepared at low substrate temperature, T_S ~220 °C. The narrow optical gap conducting material seems suitable for use in the bottom sub-cell of tandem-structured multi-junction nc-Si solar cell.

f0038
Tailoring the Performance of Phthalocyanine-Based Sensor: Side Chain Substitution and Nanofabrication
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Room temperature Cl_2 response kinetics of zinc phthalocyanine (ZnPc)-based sensor have been enhanced by peripheral substitution of alkoxy side chains functional groups on the ZnPc molecule (as Zn (II) 2,3,9,10,16,17, 23, 24-octakis(octyloxy)-29H, 31H-phthalocyanine ($ZnPcOC_8$)). $ZnPcOC_8$-based sensors have been fabricated by spin coating and solution-processed nanostructures, and Cl_2 response kinetics have been studied in the 5-1500 ppb Cl_2 concentration range. By making alkoxy substitutions at the peripheral sites of the ZnPc molecule, the detection limit of sensors is lowered from 50 ppb to 5 ppb with faster response and recovery time as compared to the ZnPc-based sensor. Among the three sensors, solution processed nanostructured sensor exhibits the best performance. The Cl_2 adsorption kinetics of sensors followed Elovich equation. The gas sensing mechanism of sensors has been investigated by XPS which suggested that the central metal ion (Zn^{+2}) of the ZnPc molecule is the preferred site for Cl_2 interaction. The present studies suggest that alkoxy substitution leads to the fabrication of highly sensitive and Cl_2 selective low-cost solution-processed gas sensors.

f0039

Effect of Concentration on the Edge-on Oriented Ordering of Spin-coated Donor-Acceptor Type Copolymer Thin Films

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The effect of concentration of polymer in solutions on the structures of spin coated poly-diketepyrrolopyrrole-thionothiophene [PDPP-2T-TT-OD] thin films were investigated using X-ray reflectivity (XR) technique. The edge-on oriented (EO) ordering near the film-substrate interface is found to be better for the film deposited with low concentration due to the lower viscosity of the solution, which has of immense importance in the device properties, as such in-plane ordering near the film-substrate interface is known to play very crucial role to get better charge transport properties in organic thin film transistor (OFET).

f0040

Chemically Modified Successive Ion by Ion Synthesis of ZnO Thin Films for Optoelectronic Applications

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Zinc oxide (ZnO) thin films are synthesized by using modified successive ionic layer adsorption and reaction techniques (SILAR) on glass substrate at room temperature. These as deposited thin films are characterized for structural, surface morphology and optical characterizations using X-ray diffraction (XRD), atomic force microscopy (AFM) and Uv-vis absorption spectroscopy. From XRD pattern; the low intensity peaks indicate that the films consist coarsely fine grains and/or amorphous in nature. The diffraction peaks observed at $2\theta = 31.71^{\circ}$, $36.27^{\circ}$and 56.29° are attributed to (100), (101) and (110) planes having hexagonal phase. Surface morphology observed from the AFM corresponds granular shape evenly distributed over substrate surface, while optical spectra attribute to exciton induced charge transportations.

f0042

Impact of 200 MeV Ag^{15+} Ion Irradiations on Structural and Morphological Properties of Epitaxial Lanthanum Nickelate Thin Films

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In this paper, we studied the influence of 200 MeV Ag^{15+} ion irradiations on the structural and morphological properties of epitaxial lanthanum nickelate (LNO) thin film on $LaAlO_3$ (001) substrate grown using PLD. The single phase and epitaxial nature of pristine as well as irradiated samples of different fluences i.e. 10^{11}, 5×10^{11} and 10^{12} ions/cm^2, were confirmed by large area 2D X-ray diffraction scans. We observed a decrease in the substrate induced lattice strain in LNO thin film with an increase in the ion dose through out-of-plane lattice constant variation using high resolution x-ray diffraction (HR-XRD). This decrease an epitaxial strain is related to irradiation induced structural defects. Further surface roughness (rms value) was found to increase with an increase in an ion dose.

f0043

Amine Functionalized Fe-MOF Membranes for Enhanced Flux and Rejection

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Here in, we report the development of amine functionalized iron based (NH2-MIL-101(Fe)) metal organic frameworks (MOF) /polysulfone polymer-based membranes for removal of chromium, humic acid and chromium-humic acid complex by dead-end filtration method. The XRD, ATR-IR, BET and FESEM studies were carried out to confirm the formation of MOF and its embedment in membranes. The contact angle shows increased hydrophilicity of MOF membrane when compared to bare membrane and the removal of pollutants increased greatly for MOF membranes.

f0044

Vanadium Pentoxide Thin Film for NO_2 Gas Sensing Application

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Present work demonstrates a synthesis of vanadium pentoxide thin film by inexpensive hydrothermal method for hazardous NO_2 gas detection. Orthorhombic crystal structure of prepared calcinated product confirmed with the help of x-ray diffraction (XRD) technique. Functional group detection was done with the help of Fourier Transform Infra-Red spectroscopy (FT-IR) and nano stick-like morphology was confirmed with the help of

scanning electron microscopy (SEM). Eventually, the gas sensing performance of vanadium pentoxide thin film was carried out for oxidizing gas NO_2. About 3.46% gas response observed towards NO_2 gas at 200°C, along with response/ recovery time 44 and 394 sec respectively.

f0045

The Effect of Electron Beam Treatment on the Third Order Nonlinear Optical Nature of the TPP Thin Film in Nano-Second Regime

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The impact of 8 MeV electron beam interaction on the third order nonlinear optical (NLO) properties of 5, 10, 15, 20 Tetraphenyl 21H, 23H- porphine (TPP) thin films were probed by means of z-scan technique with pulsed laser operating at 6 ns and 532 nm. The thin films of thickness 120 nm were fabricated using thermal vapor technique on an ultrasonically cleaned glass substrate. The irradiation sensitive UV-Visible absorption spectrum and the corresponding impact on its optical band gap were explored. The unirradiated thin film depicts reverse saturable absorption NLO property attributable to excited state absorption. A switch over to saturable absorption was observed due to the induced localized structural defects when subjected to 2.5 kGy and 10 kGy e-beam irradiation dose. The closed aperture z-scan studies illustrate self-defocusing optical nonlinearity in both pristine and irradiated thin film owing to electronic and thermal lensing effects. The strong nonlinear absorption (NLA) and nonlinear refraction (NLR) coefficient values (β and n_2) of TPP thin film provides prominence for device applications.

f0046

Effect of dc Self-bias on Residual Stress of PECVD Deposited $^{nat}B_xC$ Thin Films

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The substrate self-bias plays a significant role in determining the nature and magnitude of the residual stress in the ^{nat}boron carbide thin films deposited by Radio Frequency Plasma Enhanced Chemical Vapour Deposition (RF-PECVD) technique. The residual stress in films was calculated with the help of surface curvature method. Films were deposited as a function of substrate dc "self-bias". The stress profile in the films was found to change from tensile with a magnitude of 25 MPa to compressive with a magnitude of -150 MPa with increase of substrate self-bias from -100V to -150V.

f0047

Thermal Behaviour of Au@SiO_2 Core-shell Nanoparticles Under Nitrogen Atmosphere

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In this work, solvothermally prepared Au@SiO_2 core shell nanoparticles have been subjected to Thermo Gravimetric Analysis up to 900 °C under nitrogen atmosphere. The resulting physicochemical behavior has been explained using Transmission Electron Microscopy

analysis of the specimen before and after thermal treatment. Further, as prepared nanoparticles have also been dispersed on Si(100) substrate and subjected to high temperature annealing under nitrogen atmosphere. Interaction among Au core, SiO_2 shell, native SiO_2 and the Si substrate at high temperatures, and the resulting inter diffusion across these interfaces have been studied using Scanning Electron Microscopy.

f0048

Demonstration of strong coupling between Tamm plasmon polariton and cavity mode in metal/micro-cavity thin film multilayer

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Strong coupling between Tamm plasmon polariton (TPP) and cavity modes has been experimentally demonstrated in a metal/micro-cavity thin film multilayer. Both the TPP and cavity mode are detected as a resonant dip in the optical reflectivity spectrum. The reflectivity of the multilayer has been numerically computed using transfer matrix method. The metal/micro-cavity multilayer made of $Ag/TiO_2/(SiO_2/TiO_2)^3/SiO_2/(SiO_2/TiO_2)^4$/BK7 glass has been prepared using physical vapor deposition method. The cross-section imaging and reflectivity spectrum of the multilayer have been measured using FESEM and spectrophotometer, respectively. The measured reflectivity spectrum exhibits two resonant dips at the wavelengths of 558 nm and 584 nm, which corresponds to the coupled TPP-cavity modes resulted due to their strong coupling as predicted by the theoretical simulation. The dual resonant modes have applications in light emitting diodes, photodetectors, and optical sensors.

f0049

Growth and Structural Characterization of Copper Phthalocyanine Molecules in Thin Films

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Semiconductor organic thin films are one of the key components for modern flexible electronic devices. We have developed a thin film evaporator to deposit the organic thin films. Copper phthalocyanine (CuPc) on silicon substrate and also on cobalt thin films was deposited using this evaporator. The structural characterization of these films was done using x-ray reflectivity, and atomic force microscopy (AFM) techniques. The results show a uniform film of vertically stacked but tilted CuPc molecules on both the Si substrate and on Co/Si substrate which can be used for the study of organic spin valve systems.

f0050

ZnO Nanowires based Electronic Nose for Toxic Gas Determination

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Development of an electronic nose (EN) based on ZnO nanowires (NW) with a machine learning models namely hierarchical cluster analysis (HCA) and principal component analysis (PCA) has been demonstrated. The developed EN could successfully detect and/or discriminate toxic gases namely H_2S and NO_2 in the lower detection range from 1 to 10 ppm.

The studies revealed that the EN could qualitatively as well as quantitatively discriminate both the toxic gases under investigation.

f0052

Synthesis of Superhydrophobic/Superoleophilic Polyaniline and its Application for Oil-Water Separation

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Superhydrophobic/superoleophilic materials have attracted much attention for applications in oil/water separation owing to an extremely high water contact angle and very low oil contact angle. However, wide applications of these materials are constrained due to complex, expensive, and non-eco-friendly fabrication procedures. Here, we have successfully introduced superhydrophobic/superoleophilic properties in polyaniline using easy, simple, cost-effective, and environmentally friendly solution processible method. For this purpose, nano structured polyaniline co-doped with sodium dodecylbenzenesulfonate, are synthesized by chemical polyemeriztion method in aqueous solution. These polymer exhibit water contact angle $>150^0$ and oil contact angle $\sim 0^0$ and thus explored for oil/water separation.

f0053

Effect of O_2 Partial Pressure on Valence Band Maxima of HfO_2 Thin Film

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The effect of the oxygen (O_2) partial pressure on the valence band maxima (VBM) of pulsed laser deposited HfO_2/Si(100) thin films were investigated by photoelectron spectroscopic (PES) technique. GIXRD measurements suggest that the deposited films were in polycrystalline monoclinic phase. The VBM was determined using PES measurements. It was observed that the VBM shifted towards the higher binding energy from 2.79 eV to 3.24 eV in the film deposited in O_2 environment as compared to that deposited without O_2 environment. The O 1*s* core level spectra showed that oxygen vacancy reduces as O_2 was introduced during deposition of film. The films were found stoichiometric.

f0055

Wemple DiDomenico Single Oscillator Analysis of Zr Doped TiO_2 Thin film

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The Zr doped TiO_2 thin films are deposited on FTO glass slide by unconventional sol-gel method. The optical properties of the thin film annealed at 350^0C was studied by UV-Visible spectroscopy in the wavelength range of 300-900nm. Refractive index dispersion data is fitted with Wemple –Di Domenico single oscillator model and the various dispersion parameters are calculated. The carrier concentration to effective mass ratio and electric free carrier susceptibility was calculated by Spitzer –Fan analysis.

f0056

Electrical Characterization of $CH_3NH_3PbI_3$ Based Planar Perovskite Solar Cells

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Interface engineering between charge selective layers and photoactive metal halide perovskite absorbing layer is crucial to optimize the performance and stability of planar perovskite solar cells (PSCs). Here, we have fabricated perovskite solar cells with device architecture FTO/c-TiO_2/$CH_3NH_3PbI_3$/hole transport layer (HTL)/Ag by two step sequential spin coating method in nitrogen environment and used different conjugated polymers Poly[2,1,3-benzothiadiazole-4,7-diyl[4,4-bis(2-ethylhexyl)-4H-cyclopenta[2,1-b:3,4-b'] dithiophene-2,6-diyl]] (PCPDTBT), Poly (3-octylthiophene-2,5diyl) (P3OT) and Poly (3-hexylthiophene-2,5diyl) (P3HT), as HTL. Highest power conversion efficiency, 6.68% has been obtained owing to better perovskite/HTL interface for P3HT as HTL in $CH_3NH_3PbI_3$ based planar PSCs. Electrical characterization is performed under 100 mW/cm^2 incident solar irradiation.

f0057

Effect of substrate temperature on growth of Ti sub-oxide thin films deposited by DC Magnetron sputtering

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Amorphous titanium sub-oxide (a-TiO_x) thin films have been deposited on Si substrates by DC magnetron sputtering technique with sputter power of 50 W at room temperature (RT) and 200 °C substrate temperature (T_s). The effects of substrate temperature on the structural and morphological properties of the thin films have been investigated. All films are smooth and uniform, their density increases and thickness and roughness decrease when deposited at T_s. This work gives some idea about the growth of a-TiO_x thin films from this technique without introducing external O_2 sources.

f0059

Analysis of Varied Atmospheric Annealing Effects on the Optical Properties of an Alternative SERS Platform.

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Ameliorating the existing SERS based biosensing platforms by alternative materials focusing on cost effective, efficient and green method of approach is relevant for the present and future, where we deal with novel infections such as Covid 19. Thin films of Bismuth (Bi) were prepared on quartz substrates using DC magnetron sputtering. Post deposition annealing's were done on these films by varying atmospheric conditions. High vacuum, nitrogen (N_2) and air annealing were done at 200° C and the optical properties which supports the plasmonic enhancements were studied with comparison to the asdeposited film. The color changes noticed in the films support plasmonic responses of the fabricated Bi films and the effect of different annealing helps in concluding the Surface Plasmon Resonance's (SPR's) active responses towards optimizing a better film in future. The Surface Enhanced Raman Scattering (SERS) as an application study using Rhodamine 6G (RH6G) on initial film has resulted in an excellent upshot with Enhancement Factor (EF) of 10^5 and Limit of Detection

(LOD) of 10^{-7} molar concentration of the precursor. This confirms the potential application of the alternative films fabricated, towards developing multifunctional, wide range plasmonic biosensors.

f0060

Study On In Doped ZnO Thin Film As Electron Transport Layer For Lead Free Perovskite Solar Cells And Its Simulation

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Perovskite solar cells are new generation solar cells which show efficiency more than 20%. A perovskite solar cell consists of an electron transport layer (ETL) or a hole transport layer (HTL) between the active layer and the cathode (or the anode) in order to reduce the recombination of the free charge carriers. Indium doped Zinc Oxide (In:ZnO) thin film is a potential ETL for perovskite solar cells. In:ZnO thin film is deposited on glass substrate by chemical spray pyrolysis technique at 425 ^{0}C. Structural studies carried out using X-Ray diffractometer showed crystalline structure and the optical band gap has been calculated using UV-Visible spectroscopic technique. Hall Effect measurement of the as-deposited film showed n-type conductivity. Further, simulation using SCAPS 1D software was carried out to study the possibility of utilizing this layer as an ETL of a perovskite solar cell. The obtained solar cell structure with 3 at% indium doped ZnO as ETL has a conversion efficiency of 5.65 %

f0061

Electrical Characterization of Nickel-Oxide Based Thin Films Obtained by Chemical Bath Deposition

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In this work, Nickel Oxide (NiO) based thin film has been grown on silicon (111) substrate by chemical bath deposition method, followed by annealing at 400°C under air atmosphere. X-ray diffractometry has been used to ascertain the formation of NiO and its crystallinity. Current-Voltage (IV) characteristics have been performed at different temperatures (from 30°C to 180°C) under natural light conditions. At a constant voltage, current increases with respect to increase in temperature confirming the semiconductor nature of the NiO thin film. Further, at room temperature, the thin film shows a better current response under natural light as compared to dark conditions.

f0062

Studies on $CH_3NH_3PbI_{3-x}Cl_x$ Mixed Halide Perovskite Thin Films for Photovoltaic Application.

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Mixed halide perovskite thin films have proved to be a successful attempt to fabricate stable solar cells. We have fabricated and characterized the $CH_3NH_3PbI_{3-x}Cl_x$ mixed halide perovskite thin films for photovoltaic applications. Here, a device architecture

FTO/TiO_2/$CH_3NH_3PbI_{3-x}Cl_x$/P3OT/Ag was fabricated with TiO_2 as electron transport layer (ETL) and P3OT as hole transport layer (HTL). Structural and optical properties were investigated using X-ray diffraction, UV-vis absorption spectroscopy, and photoluminescence spectroscopy. The fabricated solar cells have been explored for P3OT as a promising hole transport material in mixed halide perovskite solar cells.

f0063

Surface modifications study of Si substrate in Ar/O_2 RF plasma for semiconductor device applications

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Plasma etching/modifications is critical in the development of silicon based electronic devices such as solar cell, integrated circuits (ICs), and transistors. In this study, we report the surface modifications of single crystalline silicon induced by RF plasma formed using argon and oxygen gases. Field emission scanning electron microscopy (FE-SEM), Atomic force microscopy (AFM) and Raman spectroscopy techniques have been utilized to examine the surface modifications. Raman spectra results reveal the enhancement in longitudinal optical phonon mode (~520.5 cm^{-1}) due to the nanostructures formation by plasma treatment. FE-SEM results analysis of the pristine and plasma treated samples indicate the surface modifications upon plasma treatment. AFM results exhibit that the surface roughness significantly increases for plasma treated sample.

f0064

The Study of Hydrophilicity, Structural and Optical Properties of Zn and N-doped TiO_2 Thin Films

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Among the wide bandgap semiconductors, TiO_2 is the highly stable and cost-efficient semiconductor used for the different photocatalysis processes like water splitting, chemical waste degradation, anti-micro bacterial activities, and more. Materials showing high hydrophilicity (surface phenomenon) with low bandgap are required to improve photocatalysis efficiency. We report the synthesis of Zn (4 wt.%) and N (4 wt.%) doped TiO_2 thin films using the spin coating technique to improve surface wettability. The XRD pattern shows the growth of the pure anatase phase of TiO_2. UV absorption spectra show a minor increment in the bandgap of the Zn and N doped TiO_2 thin films. The water contact angle with pure TiO_2 is 33.45° and reduces to 17.94° after 4 wt.% doping of Zn and N. The results show the enhanced hydrophilicity in the Zn and N doped TiO_2 thin films.

f0065

Enhanced UV Photodetection of NiO Thin Film With Au Decoration

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Nickel oxide is a p-type semiconductor having wide bandgap which makes it a desirable candidate for visible-transparent UV detection applications. In this study we have chosen the NiO thin film optimized using RF magnetron sputtering. A highly crystalline NiO thin film was achieved and tested for 365 nm UV detection. Further, when the NiO thin film was

subjected to Au decoration, the responsivity and the response time are improved by about six times.

f0066

Magnetic ground state of Iron Mononitride

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In the quest to understand the magnetic ground state of iron mononitride (FeN), we performed low energy muon spin-rotation (LE-μSR) measurements in the temperature range of 5-320 K. Instead of a rock salt (RS) type structure prevalent in transition metal nitrides, FeN crystallizes in a zinc-blende (ZB) type structure. Theoretical works suggest a non-magnetic ground state for ZB-FeN while a magnetic component has been recently observed in ultrathin (< 5 nm) FeN films. On the contrary, thicker FeN films always exhibited a nonmagnetic ground state. To further clarify, we studied 3 and 30 nm thick epitaxial FeN thin films. LE-μSR measurements confirmed the presence of a ferromagnetic component, irrespective of the thickness of FeN thin film.

f0067

Surface Morphological Study of Swift Heavy Ion Irradiated CdZnTe Thin Films

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Swift Heavy Ion (SHI) irradiation is an effective technique to induce surface modifications in thin films. In the present investigation, CdZnTe films deposited by vacuum evaporation method are irradiated by 100 MeV Ag ions at a fluence of 1×10^{12} ions/cm^2 and 5×10^{12} ions/cm^2. Atomic Force Microscopy (AFM) is employed to investigate Ag ion induced surface modifications. Effect of Ag ion irradiation on grain size, grain distribution, surface roughness, etc is studied.

f0068

Single and double layer Al and Al/Al_2O_3 passive film coatings on AZ31 alloy by PVD technique for corrosion inhibition

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This paper deals with single and dual layer coating of aluminium metal and its oxide in nanometer thicknesses on Mg alloy AZ31 to prevent the alloy from corrosion. Aluminium metal was coated on AZ31 by thermal evaporation method. On the top of that Al_2O_3 film was coated by RF Sputtering technique. Microstructure and electrochemical studies were done. Structural morphology analyzed by field emission scanning electron microscopy showed smooth, pore free and uniform film coating on AZ31. The corrosion behaviour was investigated using potentiodynamic polarization and electrochemical impedance spectroscopy carried out in wet environment of 0.6M NaCl solution. The study revealed that

the corrosion resistance was higher for AZ31 coated with 100nm thick Al film. This work provided a fascinating coating to passivate the surface of the AZ31 Mg alloy against corrosion.

f0069

Optical Characterization of CZTS Layer for solar cell application

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Copper Zinc Tin Sulphide (Cu_2ZnSnS_4) i.e., CZTS is an important quaternary semiconductor material for the third-generation solar cells. In this work, the influence of substrate temperature on the optical properties of CZTS thin films has been investigated. The fabrication route was radio frequency physical vapor deposition RF-PVD for these thin films. Spectrophotometric characterization of the films has been performed to establish a correlation between deposition parameters and optical properties of the thin film. A composite thin film of CZTS was deposited using the single target sputtering from a stoichiometric sputtering target on soda lime glass substrate. The refractive index, absorption co-efficient, band gap and thickness of thin films were calculated from measured transmission spectrum. It was found that the change in deposition temperature causes reduction of band gap from 2.05 eV to 1.9eV.

f0071

Studies on compositional and Mechanical properties of Ni-W coatings electrodeposited using citrate ammonia bath

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Ni–W alloy coatings were electrodeposited on copper and SS304L substrates using citrate bath by direct current (DC) method. The effect of bath temperature on composition, morphology and hardness of Ni–W coatings were investigated. With increase in the bath temperature from 27° C (room temperature, RT) to 90°C, the tungsten (W) concentration in the coating increased from 5.25% to 35.82 wt% and the corresponding nano hardness of the coated film also increased from 3.86GPa to 7.85GPa. Incorporation of Al_2O_3 nanoparticles in Ni–W alloy coating resulted in further increase in the hardness to 8.68GPa. The root mean square (RMS) roughness of the Ni-W-alloy film coated at RT was 128.3nm and for the film deposited at 90°C was 59.6nm. FESEM of the coated film revealed that film morphology markedly changed with deposition temperature. Ni-W alloy deposited at RT showed large grained, well faceted pyramidal microstructure and a nodular morphology for the alloy deposited at 60°C.

f0072

Understanding the structural and morphological changes in pulsed laser deposited TiO_2 thin films on soda lime glass substrates

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In the present investigation, commercially available P25 TiO_2 powder pellet is used as target for growing nanocrystalline TiO_2 thin films on heated soda lime glass substrates by using pulsed laser deposition technique (in constant EG and HV mode). XRD and FTIR characterization were studied before deposition to understand the presence of different phases and vibration modes. Two different thicknesses of the films were studied by controlling time for deposition (10 min and 30min) and keeping all other PLD parameters constant. GI-XRD of these deposited TiO_2 films were studied to understand structural/phase changes occurring in these films due to large lattice mismatch at the interface of the substrate and deposited thin film material. UV-Visible absorption was studied to understand the band edge position and to determine the band gap of these samples using Kubelka-Munk function. Surface morphological studies were carried out by using SEM to understand the growth mechanisms occurring in these films due to two different modes of depositions.

f0078

Study of Strain Relaxation in Epitaxial CrN Thin-film

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We studied the real time in-situ growth of the epitaxial CrN (001) thin-film on MgO (001) substrate using refection high energy electron diffraction (RHEED). The in –plane lattice parameter (LP) calculated from the RHEED shows rapid strain relaxation after the 5 nm of the film growth. However, the film possesses in-plane tensile strain up 30 nm which can be attributed to the very small miss-match (≈1%) between the LP of CrN and MgO. Strain in the film can be further visualized by the out of plane LP calculated from the x-ray diffraction exhibiting a compressive strain in out of plane direction. Further, the x-ray absorption spectra confirms +3 charge state of Cr and the structural transition ≈ 230 K as evidenced by the electrical resistivity measurements.

f0080

PVDF@ZnO Membrane For Their Potential Application In Oil/water Separation

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A facile synthesis of PVDF@ZnO composite membrane by cost-effective phase inversion method is reported. The samples are well characterized by XRD, FESEM and contact angle meter. XRD confirms the poly-crystalline nature of PVDF, hexagonal wurtzite structure of ZnO. Contact angle studies showed the membranes were hydrophobic-oleophilic in nature. Oil/water separation study showed that the membrane could effectively separate 96% of oily wastewater. The membranes could significantly degrade methylene blue under UV-light. Such dual functional membrane which could separate oily waste water and photocatalytically degrade organic pollutants will have potential application in sustainable cleaning of environmental pollutants in aqueous systems.

f0081

Optical and Electrical Studies on Nebulized Spray Pyrolysis coated Antimony doped Tin Oxide thin films

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Transparent conducting nanoporous thin films based on the tin oxide materials are the promising candidates for the application of electrodes, catalysts, photovoltaic devices and energy-storage devices. Antimony is a penta valance element which gives n type conductivity while doping with SnO2. Antimony doped tin oxide (ATO) thin films have been prepared by nebulized spray pyrolysis method. Electrical and optical properties were studied for the as deposited and annealed at 500°C thin films. Resistivity of the as deposited and annealed at 500°C ATO thin films were varied from 60.72 X 10–3 Ω m to 24 X 10–2 Ω m. Annealed film shows lower resistivity than the as deposited film. Both films had shown the n type conductivity which was found through the hot probe method.

f0082

Poole-Frenkel Conduction Mechanism Observed in Sputter Grown Silicon Carbide Thin Film

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SiC thin film based devices are in great demand because of their better performance at high temperature, high frequency and high power applications. Here, SiC films are fabricated by a cost-effective and simple approach of RF magnetron sputtering. Metal-Semiconductor-Metal (MSM) junction is fabricated using gold electrodes by shadow sputtering. The Current-Voltage (I-V) characteristic of this fabricated device reveals the presence of Poole-Frenkel mechanism at Gold-SiC MSM junction indicating defect states and trap centers, which can be advantageously used to design some specialized electronic devices for application such as optical detection, power electronics, memory and energy-efficient devices.

f0083

Study of Intense Ion Beam Interaction Effect on Post-Experimental Nuclear Reaction Thin Film by SEM Investigation.

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It has been observed that material properties tend to undergo changes under passage of energetic beams. The MeV-range energetic ions beyond Coulomb's barrier of a target-beam combination lead to nuclear reactions, subsequently the modification of target materials. In other terms, this can be understood to be consumption or high burn up, yielding reaction fragments to the surrounding. Lanthanum Erbium (Er) is used as burnable neutron absorbers with nuclear fuel. In this study we have reported the surface morphology of selected targets Te, Er, Tm, Sn and Zn exposed to MeV ion and to have local high burnup conditions. The permanent morphological structures mentioned below are observed 1. Elongated and

vermicular inter-granular bubbles in Te. 2. Clustered spherical inter-granular bubbles and fuel cracks in Er and Tm. 3.Carbonaceous deposits on Sn and Zn.

f0084

Synthesis of High-end Piezoelectric and Electroactive Polymer Nanocomposite Thin Films based on PVDF/CNTs for Ultrasound Transducer Application.

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A suitable PVDF/CNTs nanocomposite based high-end piezoelectric and colossal dielectric material is developed through simple low-cost drop casting and high voltage electro poling methods. The transformation of nonpolar α–phase to polar and electroactive electroactive β–phase was observed and quantified by FTIR spectra and, XRD diffraction pattern. Highest piezoelectric β – phase exhibited 85.2 % in PVDF/CNTs nanocomposite thin film. This enhancement of polymer composites thin film's β–phase also shows the high dielectric constant ~ 64 at 20 Hz. Same piezoelectric thin film is used to fabricate a high frequency, low pressure sensitive ultrasound senor which converts ultrasound pulsing waves generated by 10 MHz ultrasound transducer to an electrical output (~70 mV).

f0086

Study of thermal oxidation behavior of N+ ion implanted zirconium thin film

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Zirconium thin films were deposited on sapphire substrate using DC magnetron sputtering at room temperature and in argon atmosphere. These thin films were implanted with nitrogen ion beam and further annealed to study the oxidation behavior. As expected, XRD reveals that the samples completely turned to ZrO_2. The band gap of the film is found to be 3.15 eV from diffused reflectance spectroscopy. SEM analysis shows a peculiar nature of the N^+ ion implanted and annealed thin film where blisters are formed and also there are cracks developed on the blisters for the release of implanted nitrogen. The Zr film which was annealed at nitrogen atmosphere retained the metallic luster and SEM shows a smooth film with large grain boundaries without any blisters.

f0087

Magnetic Proximity Effect In $La_{0.67}Sr_{0.33}MnO_3$ /$SrTiO_3$/$YBa_2Cu_3O_{7-\delta}$ Heterostructures

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Magnetic proximity effect (MPE) in $La_{0.67}Sr_{0.33}MnO_3$(LSMO)/$SrTiO_3$(STO)/$YBa_2Cu_3O_{7-\delta}$(YBCO) heterostructures has been investigated using spin-polarized neutron reflectivity experiments. We find modulation in magnetization in the ferromagnetic LSMO layer at the

interface in the form of an emergent layer of thickness ~ 20 Å with depleted magnetism. This emergent layer is found only below the superconducting transition temperature of YBCO, indicating that superconductivity is essential for the phenomenon of MPE which is attributed to tunnelling of electron cooper pairs from YBCO to LSMO through the STO layer.

f0088

Highly Sensitive Room Temperature NO_2 Gas Sensor Based on MgO Functionalized ZnO Nanowires

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In recent years, surface modification of metal oxide semiconductors have been found to significantly improve their gas sensing behaviour. In the present study, sensing performance of binary heterostructure formed between ZnO NWs and MgO have been investigated . Sensor film was fabricated by employing facile hydrothermal method for nanowire growth over which thin layer of MgO was deposited using electron beam evaporation. The sensing characteristics of the fabricated films were examined and compared at different working temperatures. It has been observed that MgO functionalization remarkably improves the sensor response towards NO_2 gas with (R_g/R_a ~ 310) for 10 ppm conc. at room temperature with minimum detection limit of 400ppb. Compare to pristine ZnO NW film, 25 fold increase in sensor response was achieved in composite films at room temperature with highly selective and stable behaviour. Enhanced response observed in case of composite film could be attributed to synergistic effects of ZnO and MgO.

f0089

Thickness dependent crystallinity variation in ZnO thin films synthesized by pulsed laser deposition method

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ZnO thinfilms were synthesized by pulsed laser deposition technique on Silicon substrates at various thicknesses. The influence of film thickness on crystallinity of the film was analyzed via fracture cross-sectional SEM and GI-XRD techniques. SEM observation revealed the columnar grain structure with orientation vertical to the substrate. XRD analysis revealed the preferential orientation along c-axis of the films. The preferential orientation improved with the thickness. RMS roughness of the films measured by AFM technique initially increased with thickness and decreased afterwards for higher thickness

f0090

Hydrogen-induced modification of opto-electronic properties of ZnO(10-10)/graphene interface

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Organic and inorganic interfaces are known to offer hybrid functionalities which are superior to that of individual materials. However, the unavoidable adsorption of gas molecules can

further modify the opto-electronic properties in devices. In this work using first-principles calculations, we systematically investigated the role of H on opto-electronic properties of the ZnO/Graphene heterostructure. Our findings indicate that the direction of charge transfer in the interface depends on the presence of H and therefore presence of metallicity in ZnO. A band gap opening of 0.07 eV in graphene is observed due to H adsorption, this is primarily because of strain developed on graphene. A significant enhancement to optical absorption coefficient along with wide absorption wavelength range in the visible light region. This is due to H adsorption. This can be useful in the fields of optical sensors, photo detectors, and solar cells.

f0091

Tuning of electronic and magnetic properties $SrRuO_3$ thin film via electric field assisted growth

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Electric field assisted and unassisted $SrRuO_3$ thin films have been grown on the (*00l*) Si substrate using pulsed laser deposition technique. An applied electric field during film growth enhances the nuclei coalescence, resulting a better crystallinity of film. X-ray absorption study suggests that in electric field assisted film, the crystal field splitting is found higher as compared to unassisted SRO film, resulting the enhanced Ru 4*d*- O 2*p* hybridization. Enhanced magnetic anisotropy is observed in electric field assisted $SrRuO_3$ thin film.

f0092

Study of Interfaces in Metal/ C_{60} Bilayer under X-ray Standing Wave Condition; Theoretical Simulations

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In the present work, we demonstrated the depth selectivity of FeCoB/C_{60} interface on basis of theoretical simulations by generating x-ray standing wave (XSW) using a waveguide structure Si/Pt/ C_{60}/ FeCoB (interface)/ FeCoB (bulk)/ C_{60}/Pt. Fe- k_α fluorescence (XRF) spectra were simulated theoretically for increasing angle of incidence for the different values of electron density and thickness of interface FeCoB layer. It is found that the fluorescence peaks corresponding to the XSW antinodes crossing the interface layer is highly sensitive to the electron density and thickness of interface FeCoB layers. Present study demonstrates that by measuring electron density profiles through XRF measurement under XSW, Interface resolved structural information can be achieved by moving antinode region and selecting appropriate incident angle.

f0093

Morphological Evolution and Surface/Interface Fe-oxide formation in Epitaxial Fe(001)/MgO(001) Thin Film

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Epitaxial Fe film has been grown on ion beam sputtered MgO(001) substrate by electron beam evaporation. Reflection high energy electron diffraction (RHEED) and transport

measurements (TM) were performed simultaneously during the growth of the film. While TM provided information about film morphology, RHEED provided information about the structure of the film. The film grows via Volmer–Weber mechanism, where epitaxial islands grow larger to impinge with other islands and eventually coalesce into a continuous film at around 1.8 nm thickness. In contrast to the literature, no evidence of the formation of the iron oxide layer is observed at Fe/MgO interface even up to 300°C. High quality epitaxial Fe_3O_4 layer is found to develop on Fe surface when the sample is annealed under a moderate oxygen partial pressure.

f0094

Optical Properties of $La_{0.7}Sr_{0.3}MnO_3$/ZnO Heterostructures

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$La_{0.7}Sr_{0.3}MnO_3$/ZnO heterostructures of various ZnO thicknesses have been grown on (001) oriented Si substrate using RF magnetron sputtering. The growth conditions of the $La_{0.7}Sr_{0.3}MnO_3$ and ZnO were chosen to achieve the stoichiometry and the preferential growth along the *(00l)* direction. The variation of band gap of ZnO with thickness has been determined using diffuse reflectance spectroscopy. The band gap of ZnO grown on Si/LSMO increases with decrease in the thickness of the ZnO films. The band structure of bulk ZnO, hence, the band gap was studied using the first-principle density functional theory. This LSMO/ZnO heterostructures can be utilized for a wide range of spintronics and optoelectronics applications**.**

f0095

Fabrication Of CuO Coated Mesh For Efficient Oil/Water Separation

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In this work, we fabricated CuO coated superhydrophobic mesh by simple immersion method. The coated mesh showed excellent superhydrophobic-superoleophilic mesh with water and oil contact angle of 156° and 0° respectively. The as deposited mesh meets the current need for the separation of oil-water mixtures owing to its high separation efficiency (~98%) and stability.

f0096

X-ray absorption study of manganese mononitride thin films

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We report a comprehensive study to resolve the debate about the crystal structure of manganese mononitride (MnN). Single phase MnN thin film was obtained by varying the partial pressure of N_2 in the sputtering process. The optimized film was studied in detail using x-ray absorption near edge spectroscopy at Mn and N *K*-edges and Mn *L*-edge. Pre-edge peak intensity of XANES at metal *K*-edge is very sensitive to the local coordination symmetry of the central atom and was used to confirm the crystal structure of MnN thin film.

g: COMPUTATIONAL METHODS, AND ELECTRONIC STRUCTURES

g0001

DFT+U Study on the Half-Metallic Ferromagnetic Behavior in CoRuVAl Quaternary Heusler Alloy

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In the framework of density functional theory, the physical characteristics of the quaternary Heusler alloy CoRuVAl have been estimated using the Full Potential and Linearized Augmented plane wave (FP-LAPW) approach. We employed a Coulomb interaction (U) within the GGA method to get accurate results. The electronic structure has half-metallic behavior, and a minority band gap of 0.278 eV is formed at Fermi level. By satisfying the Slater - Pauling rule of 24 (M_t=Z_t-24), we estimated a total magnetic moment of 1 μ_B. The calculated results show that CoRuVAl quaternary Heusler alloy is a good spintronics material.

g0002

***Ab initio* investigation of the electronic structure and magnetic properties of cubic spinel Fe_3O_4**

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We present the results of *ab initio* calculations of cubic Fe_3O_4, investigated by using density functional theory (DFT). The computed density of states (DOS) shows the distribution of cations in the octahedral sites give rise to half-metallic behavior. The magnetocrystalline anisotropy energy (MAE) computed by both the total energy calculations and magnetic force theorem are equal to -2.92×10^4 J/m^3 and -2.02×10^4 J/m^3 respectively comparable to the experimentally observed value of -2.0×10^4 J/m^3.

g0003

Importance of The Type Of Coulomb Interaction In DFT+DMFT Method To Study Magnetic And Electronic Properties of Nickel

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Here, the effect of different Coulomb interactions is investigated within DFT+DMFT method for exploring the magnetic and electronic structure properties of Nickel (Ni). The value of U =7.2 eV (J=1.2 eV) is used for this study, which is computed by cRPA (Yukawa screening). The results of the comparative study of estimations by Coulomb interactions show that Full type of Coulomb interaction gives T_c (~600K) in close approximation with experimental value (631K). The value of saturation magnetization using Ising (Full) comes out to be ~0.50 (~0.44) μ_B/Ni. Momentum-resolved spectral function using both Coulomb interactions is also studied and the results suggest considerable dependence of the physical properties on the type of Coulomb interaction used. Thus, using the appropriate Coulomb interaction to examine the physical properties of materials becomes crucial in the DFT +DMFT framework.

g0004

The First-Principles Calculations of Structural, Elastic, Electronic, and Magnetic Properties of Ru2TiMn Heusler Alloy

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Structural, elastic, electronic and magnetic properties of novel Ru_2TiMn (RTM) Heusler alloy have been investigated by using the first principles calculations based on the framework of density functional theory (DFT). The elastic constants, Cij, elastic moduli, mechanical stabilities and the Raman spectrum of RTM have been estimated. The metallic ferromagnetic behavior of RTM has predicted with the approach of GGA-PBE and GGA+U-PBE and a comparative study of electronic density of states (DOS), projected density of states (PDOS), band structures have been analyzed. To the best our knowledge, physical properties of RTM have neither measured experimentally nor calculated theoretically leads to the scope of future experimental study on Ru_2TiMn.

g0005

Modelling of Shock-Hugoniot for single crystal Ni using Molecular Dynamics : Comparison with ab-initio and Experimental results.

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Molecular Dynamics (MD) simulations and ab-initio calculations have been carried out to obtain the coefficients of the linear relation between the shock velocity (U_S) and particle velocity (U_S) for single crystal, Nickel (Ni). Foiles embedded Atom Method (EAM) potential is used in the MD simulations. In order to confirm the effectiveness of Foiles EAM potential for high strain rate and high pressure shock simulations, the results from MD are compared with both, the ab-initio calculations and published experimental results. Our simulations yields a better match with experiments, compared to earlier published MD results.

g0006

Applicability of Oseltamivir Drug against SARS-CoV-2:A Computational Study

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The virus SARS-CoV-2 has created an epidemic situation all over the world from the last year. Presently, the researcher and expert groups have suggested a number of variants of COVID-19 and they labelled them as α, β, γ, δ, and δ+. δ+ variation appears to spread more quickly and easily than other variants, which potentially leading to an increase in COVID-19 cases, which is suggested as the most devastating variant. In the present study, we have tested the efficacy of antiviral drug Oseltamivir against COVID-19. The strong binding affinity, hydrogen bond interaction and lower inhibition constant validated the better complexation possibility of O:3CL^{pro} structure. Various thermodynamical parameters from

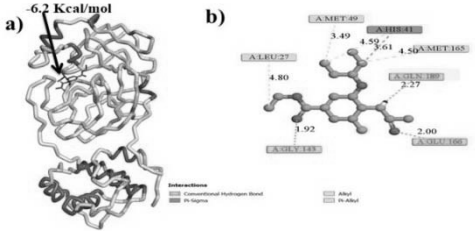

Fig 1: a) Binding energy **b)** Possible types of interaction in pose obtained from O: 3CL^{pro}

Molecular dynamics (MD) simulations like RMSD, RMSF, SASA energy, interaction energies, Gibbs free energy (ΔG_{bind}) etc. also favoured effectivity of Oseltamivir (O) against CoV-2 protease. We are definite that our in-silico results on the drug Oseltamivir against CoV-2 infections will help the current clinical research to identify the perfect cure for COVID -19 treatments.

g0007

Energy Loss Rate in Bilayer Graphene on GaAs Substrate due to Piezoelectric Phonon Scattering

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Electron excitation and subsequent electron energy loss rate by scattering through piezoelectric acoustic phonon modes in bilayer graphene from piezoelectric GaAs substrate at a distance apart have been studied as a function of elevated temperature, substrate distance, and the electron density in the Equipartition regime. A recent study has reported the energy loss rate in the conditions mentioned above in the Bloch-Gruneisen regime, which corresponds to the low-temperature region depicting T^3 dependency on temperature and $n^{-3/2}$ on electron density. The electron-phonon interaction at high temperatures is vital in determining the novel thermoelectric properties of low-dimensional materials. Motivated by this, we investigated electron-piezoelectric acoustic phonon scattering and obtained analytical results for the electron energy loss rate at high temperatures. We find the electron energy loss rate to vary linearly with temperature, d^{-2} with substrate distance and as $n^{-3/2}$ with electron density.

g0010

Computational analysis of Ethyl N-acetyl-L-Tyrosinate (ENALT) by DFT calculations for NLO applications

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The theoretical investigation on the Ethyl N-acetyl-L-Tyrosinate (ENALT) molecule was studied for nonlinear optical (NLO) applications by quantum chemical calculations. The geometrical structure optimization and Mulliken charge distribution were obtained through DFT-B3LYP/6-31G (d,p). The theoretical IR spectra was analyzed for fundamental vibrations and fingerprint of the molecule. The frontier molecular orbitals and hyperpolarizability value are computed and confirm that the ENALT molecules have higher NLO property.

g0011

HAXPES Study of a Kondo Lattice System $CeCuAs_2$

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We investigate the electronic properties of a Ce-based Kondo material, $CeCuAs_2$. To probe the surface bulk differences of the electronic structure, high-resolution hard *x*-ray photoemission spectroscopy measurements were done with photon energies having varying probing depth. We observe significant difference in the hybridization physics for the surface and bulk electronic structure leading to different Ce valencies. Surface termination appears to play an important role in the correlation physics of this system. Spectra show signature of electron-plasmon coupling induced loss features. These results bring out complexity of a novel Kondo material having no magnetic order down to the lowest temperature studied and have significantly different surface-bulk properties.

g0012

First-principles study of Co and Ho co-doped ZnO

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In this work from first-principles simulations, we investigate the structural, electronic, and magnetic properties of transition metal cobalt (Co) and rare-earth holmium (Ho) co-doped zinc oxide (ZnO) using Quantum-Espresso. A lot of interesting results were found from the analysis of energy band structure and density of states. From spin-polarized calculations within the framework of density functional theory, we have noticed that the value of total magnetization of co-doped ZnO is substantially enhanced compared to that of pure ZnO.

g0013

Electronic and Optical Properties of Single Benzene Ring Graphene Quantum Dot

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In the present work, we have investigated the structural, electronic and optical properties of Graphene Quantum Dot (GQD) containing single benzene ring in strong confinement regime using Density Functional Theory. HOMO and LUMO energy gap of this single benzene ring GQD is found to be equal to 7.23eV which is very close to the band gap predicted by Goki Eda et al. The Density of States (DOS) of this QD are found to be discrete which is very well known property of QDs. Further, the absorption coefficient and imaginary part of dielectric function for this single benzene ring GQD is calculated for parallel and perpendicular polarizations. The plasma frequency (Ω) emerges at position 5eV for parallel polarization. However, for perpendicular polarization there is occurrence of two plasma frequencies nearly at 13.7 eV and 17.6 eV.

g0014

Silver adsorption on monolayer MoS_2 and WS_2: A first principles study

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First principles calculations based on periodic boundary conditions were carried out using density functional theory (DFT) to obtain the structural and electronic properties of Ag

adsorbed MoS_2 and WS_2 monolayers. The results demonstrate emergence of in-gap states due to Ag adsorption on the monolayers of MoS_2 and WS_2, thus, proposing a simple method of modification of the electronic properties and tuning the bandgap of these monolayers. The appearance of additional states within the bandgap can be observed near the Fermi energy as a result of the contribution from Ag s and Mo d orbitals.

g0015

Optical Properties Of Two-Dimensional Pentagonal Tellurene

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Motivated by the simple structures and astonishing properties of mono-elemental monolayers of group VI-b elements, the electronic and optical properties of newly predicted pentagonal tellurene (penta-Te) have been studied with the help of density functional theory. It has a pentagonal structure constituting six tellurium atoms with a square unit cell. The indirect band gap of 0.89 eV has been obtained with PBE functional. The absorbance peaks of optical spectra lie in the UV-visible region imply its optoelectronic applications. Comprising the semiconductor nature, previously examined mechanical and thermoelectric (TE) properties, and optoelectronic (OE) properties, this material has potential applications in flexible OE-TE multifunctional devices.

g0016

Collinear Magnetic Coupling of 3d Transition Metal Atoms on Ni_2MnGa (001) Surface

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In this paper, we focus on magnetic 3d atoms, used as an adatom on the Ni_2MnGa(001) surface. We investigate the orientation of the magnetic atoms and stabilization of collinear magnetic solutions of these composite systems. It is found that early transition metals (Ti,V,Cr,Mn) couple anti-ferromagnetically to the substrate, while (Fe,Co,Ni) couple ferromagnetically (FM). Further, surface and termination dependent magnetic coupling of lattice matched Fe have been studied and it is observed that Fe has FM coupling to the substrate as well as within themselves irrespective of Fe layer thickness and surface termination.

g0017

Correlation Effects In Finite Width One-Dimensional Electron Wire

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We study the ground state properties of the electron fluid in one-dimension at high density. The regularization of the Coulomb potential in one-dimension is achieved by confining the electron in one-dimension through a harmonic potential. The dependence of the ground state energy on the wire width is studied for electron fluid at high density confined in a Harmonic potential using the variational quantum Monte Carlo simulation. The low energy physics of Tomonaga-Luttinger liquid are characterized by Tomonaga-Luttinger parameter or exponents. We have extracted the Tomonaga-Luttinger liquid exponent from the momentum

density data by fitting the data around k_F for different confinement of harmonic wire widths. The Tomonaga-Luttinger liquid exponent is than extrapolated to the infinitely thin wire. The extrapolated Tomonaga-Luttinger liquid parameter is in agreement with the infinitely thin wire simulation data.

g0018

Structural and Electronic Properties of WS_2-MoS_2 Van Der Waals Heterostructures

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Van der Waals heterostructures, which are created by stacking monolayers vertically, have a wide range of optoelectronic applications. The structural and electrical properties of heterobilayer WS_2-MoS_2 Transition Metal Dichalcogenide are explored using first principle calculations. According to our calculations, the monolayers MoS_2 and WS_2 have direct bandgaps. However, when these monolayers are stacked vertically to form a heterobilayer with van der Waals interaction, we get indirect bandgaps with bandgaps smaller than those of the monolayers WS_2 and MoS_2.

g0019

Electronic and Optical Properties of Novel Double Perovskite Compound Cs_2RbInI_6

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Novel energy materials grab the much attention of researchers because of the huge demand for green energy sources. Double perovskites of $A_2BB'X_6$ framework has been conspicuous by the dint of their magnificent electronic and optical properties. We have computed the physical properties of Cs_2RbInI_6 double perovskite compound using first principle method along with density functional theory (DFT). Complete computational analysis has been done within wien2k code. Cs_2RbInI_6 demonstrates the low band gap, high absorption and high dielectric constant which are preferable for various optoelectronic applications.

g0020

Introduction of Defects in 2D α-SiN for Improvement in Hydrogen Evolution Reaction Activity: A DFT Study

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In this work, we have studied the potential of pristine and defected 2D α-SiX for HER catalyst. The defect enhances HER activity by 90% as compared to pristine α-SiN and makes it comparable to one of the best Pt metal alloys. The enhanced performance of HER is attributed to the redistribution of charges after vacancy defect creation. Defect makes α-SiN metallic which serves as an electrocatalyst. This work could open up an avenue for the fabrication of earth abundant non-nobel metal based electrocatalyst.

g0022

The Magnetic Order And Electronic Structure Of Gd Doped $EuCd_2As_2$

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In this work, we have theoretically investigated the magnetic order and electronic structure of $Eu_{2/3}Gd_{1/3}Cd_2As_2$ compound. The chemical substitution at $1/3^{rd}$ of Eu sites in $EuCd_2As_2$ by Gd is observed to affect significantly its physical properties. Our density functional theory (DFT) calculations reveal that Gd substitution leads to a transition from semi metallic antiferromagnetic (A-AFM) ground state of the parent compound to metallic ferromagnetic ground state, where the energy difference between FM and A-AFM configuration is quite close, which can be tuned easily with externally applied magnetic field.

g0023

In-situ STS studies and first principles calculations on the mechanically exfoliated WS_2 layers

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Transition metal dichalcogenides (TMDs) have received immense research interest in the past few years due to their promising applications in nano- and opto- electronic devices. In the present work, we report mechanical exfoliation of few layers of ultra pure WS_2 crystal under ultra-high vacuum (UHV) conditions and investigation of the local electronic structure by in-situ scanning tunneling spectroscopy (STS) measurements and first principle calculations. STS investigations reveal the local density of states of the WS_2 surface with a bandgap of approximately 1.34 eV. First principles calculations performed on the bulk WS_2 crystal corroborate the experimental STS results with an indirect bandgap of the order of 1.38 eV and evidence of S *p* and W *d* states at both sides of the Fermi level.

g0024

$(ZnO)_{60}$: An UV active magic nanocluster under DFT study

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The minimized energy geometries of $(ZnO)_{6n}$ (n= 8 to 11) clusters were optimized using a systematic density functional theory. In addition to our previously identified magic nanocluster ($(ZnO)_{42}$, the present work reports a novel ultraviolet active magic nanocluster $(ZnO)_{60}$. $(ZnO)_{60}$is identify as exceptionally stable 'magic' nanocluster upon investigation on the electronic properties of $(ZnO)_{6n}$ nanoclusters in terms of the HOMO-LUMO gap (HLG), ionization potential (IP), electron affinity (EA), chemical hardness (η), electrophilicity index (ω) and energy gain (ΔE). Interestingly, as the n value increases in the multiple of six, the electronic properties energy gain (ΔE) of ZnO clusters demonstrate a

zigzag pattern, identifying 'magic' $(ZnO)_{60}$. Furthermore, the optical absorption spectra analysis show $(ZnO)_{60}$is active in the UV-A region. The developed magic nanocluster in the present work is expected to find useful applications as quantum dots and cluster assembled materials in semiconductor and optoelectronics domains.

g0026

Prediction of Intrinsic Spin Half-Metallicity and Ferromagnetism of Co-based Full Heusler Alloys: Hunt for Spintronic Applicability

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The computational methods are reliable in predicting the ground state as well as other properties of a material. There have been abundant endeavors to configure the high spin-polarized materials for controlling the spin electron to renovate conventional electronics. In the light of current investigation, the structural stability as well as magneto-electronic properties of Co-based Heusler alloys has been examined. The structural optimization signifies that both the materials are most stable in the ferromagnetic phase. The present Heusler alloys deliver half metallic performance conveys 100% spin polarization at Femi level. The source of carrying magnetism generates predominantly from half-filled *d*-orbitals of the present set of Co-based Heusler compounds. The present set of Co-based Heusler materials reflects good performance in spintronics applications.

g0028

Modelling the reactivity of Entrectinib and evaluation of its potential anticancer activity using Molecular Docking approach

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Hepatocellular carcinoma is a type of adenocarcinoma and the most common type of liver tumor that leads to approximately 80% of deaths due to cancer worldwide. More than 600,000 people die of HCC each year. A proper drug is necessary to fight against it in the initial stages as the disease can't be cured in advanced stages and need organ implantation. The research on this disease needs to be augmented. The advancement is needed in both the medical and pharmaceutical fields, for finding and synthesizing a proper drug for curing HCC. Drug repurposing has been a trending method in the medicinal industry that has given positive results for many diseases. On the other hand, Entrectinib (ENC) is a used as an anticancer drug for the treatment of ROS1-positive non-small cell lung cancer. Thus, for the present study, ENC has attracted much attention to be used as an effective repurposed drug. For checking the potentiality of ENC as a repurposed drug against HCC, we have reported the structure, charge and molecular electrostatic potential analysis to check the reactivity and stability of the ENC molecule with the help of Density functional theory. Spectral analysis (UV-Vis analysis) is also mentioned to check the electronic stability of the probe molecule. To validate the candidature of ENC as a repurposed drug, Molecular docking is also performed for ENC with vascular endothelial growth factor (VEGFR-2) to report the mechanism of ENC as an anticancer agent. The good chemical reactivity and docking scores are obtained for ENC suggesting that the molecule is chemically stable and can be used as a potent druglike molecule against various HCC drug receptors.

g0029

Investigation of Nonlinear Optical Response of Organic Compound Pyrrolidine-2,5-dione

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Nonlinear optical (NLO) materials have wide applicability in the field of material science and engineering. In the past decades, the NLO have become wide interdisciplinary field of research. These are used in electro-optical modulation, dynamic holography, lasers, telecommunications and photonic devices, etc. These materials have asymmetrical geometries due to which electron cloud delocalized between donor and acceptor moieties. These materials produce altered phase, when interacts with high electromagnetic fields. NLOs are classified as organic and inorganic depending on the source of the extraction of the material. However, with better NLO responses and various other features like cheap, easy availability and easy synthesis makes the organic NLOs more preferrable than the inorganics one. In the present work, the computational investigation has been done for detecting NLO responses of an organic compound pyrrolidine derivative. Pyrrolidine-2,5-dione (P2D) is optimized to ground state energy level by B3LYP/6-311G basis set using density functional theory (DFT). Optimized geometry is used for determining the Mulliken charges, and molecular electrostatic potential (MEP) surface. Frontier molecular orbitals (FMO) are also calculated to determine the parameters like energy gap (ΔE), ionization potential (IP), electron affinity (EA), chemical potential (CP), and electronegativity (χ). Spectral behavior and the high value of dipole moment (μ_{total}), polarizability (α) and first order hyperpolarizability (β) shows the high polarizable nature of P2D. All these properties suggested that the probe molecule may indeed have the possibility to show good NLO behaviour.

g0030

Structural and Electronics properties of the RhFeSi Compound under different Approaches

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Investigation of the structural and electronic properties of the RuFeSi has been performed using the first principle calculations. The optimized lattice parameters of the system corresponding to the ground state has been determined using the Murnaghan's equation of states. The positive phonon dispersion predicts the dynamical stability of the alloy. To account for the highly correlated valence electrons, an onsite Coulomb interaction (*U*) is included in local density approximation (LDA) and generalized gradient approximation (GGA) as LDA+*U* and GGA+*U,* respectively. Within LDA+*U* and GGA+*U* schemes, the title material reflects half-metallic behavior with a band gap of 0.81 eV under both the schemes.

g0032

Structural, Electronic and Magnetic Properties of Three Filled Skutterudites $Nd_xSm_{1-x}Fe_4Sb_{12}$ (x = 1, 0.5 and 0)

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Structural, electronic and magnetic properties of three filled skutterudites $NdFe_4Sb_{12}$, $Nd_{0.5}Sm_{0.5}Fe_4Sb_{12}$ and $SmFe_4Sb_{12}$ have been studied using density functional theory. Optimized lattice constants are found to be 8.9673 Å, 9.1564 Å and 9.1461 Å respectively. The electronic band structure and DOS show the half metallic behaviour of the doped material with effective magnetic moment 6.00 μ_B whereas the two pure systems exhibit metallic and weakly ferromagnetic nature.

g0033

Electron and phonon properties of α-Uranium from first principles simulations

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α-Uranium displays Kohn anomaly in multiple phonon branches at charge density wave (CDW) wavevector $\mathbf{q}_{CDW}$ above the CDW transition. The Kohn anomalies are reflected in calculated phonon dispersions as sudden dips and unstable phonon branch(es) at $\mathbf{q}_{CDW}$. As shown in literature for 2H-$NbSe_2$[1], increasing electron smearing (indirectly electron temperature) in density functional theory calculations can stabilize unstable phonons arising due to the Kohn anomalies. We perform first-principles simulations on α-Uranium with a similar approach to obtain stable phonon dispersion. However, we find that phonon branch(es) remain(s) unstable at $\mathbf{q}_{CDW}$. Moreover, we calculate electrical conductivity and Seebeck Coefficient due to electron-electron scattering within constant relaxation time approximation and compare with available experimental data.

g0034

The Mn K-edge EXAFS studies of Co_2MnAl

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We have investigated the local structure around the Mn site in Co_2MnAl Heusler alloy using Mn K-edge Extended X-ray Absorption Spectroscopic (EXAFS) technique. The polycrystalline sample of Co_2MnAl was prepared by arc melting method and characterized by X-ray diffraction (XRD) and field dependent magnetic measurements. The XRD result shows that the compound stabilizes in B2 cubic structure with lattice parameter 5.76 Å**.** The field dependent magnetic measurement gives a saturation magnetic moment of 4.20 μ_B/f.u. which is nearer to the expected value for the B2 phase. EXAFS analysis suggests the local environment around the Mn site is different from the global structure as revealed by XRD.

g0035

Enhancement of Adsorption Performance of NH_3 Gas Molecule towards Cyclo[18]Carbon: An Effect of Substitutional Doping

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In this work, we have studied the potential of the pristine; B and N doped C_{18} nanocluster for toxic NH_3 molecule adsorption. We have evaluated the structural change, adsorption energy, electrical conductivity and recovery time to understand the effective sensing mechanism. B and N doping modulated the electronic properties of C_{18} nanocluster. After B and N doping E_G is reduces to 6.15 eV and 4.72 eV from 6.74 eV. The large adsorption energy and drastic change in electrical conductivity after NH_3 gas molecule adsorption over B doped C_{18} nanocluster indicates very strong interaction between them. Recovery time calculations suggest that B doped C_{18} nanocluster can be used as NH_3 gas molecule remover from specific environments.

g0036
Pressure Induced Topological Phase Transition in c-YN
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We present a first-principles based analysis of quantum phase transition in cubic (*c*)-Yttrium Nitride. We propose that the *NaCl-type* YN can host a topological phase transition under applied hydrostatic pressure, in the presence of Spin-orbit Coupling (SOC). Under ambient conditions, YN is an insulator but it shows topological phase transition at Gamma point under the external pressure of 20 GPa without breaking any symmetry. The topological phase transition pressure (20 GPa) is much lower than the structural phase transition pressure (170 GPa) for YN.

g0037
Prediction of Two Dimensional Wide Bandgap Semiconductor $PbBr_2$ Monolayer Using First Principle Calculations
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The wide bandgap semiconductors can be used as high temperature electronic devices, RF signal processing, visible range light-emitting diode application, and many more. Two-dimensional wide bandgap semiconductor material $PbBr_2$ has been predicted using density functional theory. Monolayer $PbBr_2$ has hexagonal structure with space group 164 (P-3 m1). The unit cell consists of two Br atoms and on Pb atom and lattice constant of its relaxed structure is a=b=4.49Å. A positive phonon dispersion curve suggested the dynamical stability of the material. The band structure indicates that it's an indirect bandgap semiconductor with bandgap of 2.74 eV. On application of biaxial strain, the bandgap increases with tensile strain and decreases with compressive strain. From 10% to -10% applied strain the material shows indirect semiconducting properties. From 10% to 0% applied strain the CBM rests at Γ point and VBM rests at K point while on application of negative strain from -2% to -8% the VBM shift between K and Γ point. At -10% strain the CBM shift to high symmetric M point while VBM rests between K and Γ point.

g0038

Defects Optimization For Efficient All Inorganic $CsPbI_2Br$ Perovskite Solar Cell

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All-inorganic perovskite solar cells recently attracted the scientific community for their excellent stability over hybrid organic-inorganic based perovskite solar cells. Their performance is, however, not high as of organic or hybrid counterparts. Here we simulated fully inorganic $CsPbI_2Br$ based perovskite solar cells using SCAPS-1D software. Since defects at perovskite bulk material and the interface of perovskite play a vital role in the performance of perovskite solar cells, we suggested the fair value of defect density at perovskite bulk to be 10^{15} (cm-3) and for perovskite interfaces to be 5×10^{17} (cm-3) to be efficient perovskite solar cells. This work paves the way to develop highly efficient all-inorganic $CsPbI_2Br$ perovskite solar cells.

g0039

Molecular Dynamics Simulation of Primary Radiation Damage in Tungsten using Two-Temperature Model

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Molecular Dynamics simulations have been performed to assess the primary radiation damage that occurs in Tungsten using an electronic stopping model called Two-Temperature Model (TTM). There are other electronic stopping models available like Lindhard-Scharff (LS). In this study, we perform high energy MD simulations in Tungsten and compare the results of TTM model with MD results of LS model and also compare the results without considering electronic stopping.

g0040

Effect Of Strain On Electronic And Optical Properties Of The Lead Free Photovoltaic Material $Cs_2AgInBr_6$: DFT Study

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Recently the double perovskite (DP) $Cs_2AgInBr_6$ is reported to be the prominent solar absorber material due to its direct nature of band gap value of 1.33 eV lying in the visible region. It emerged as potential alternative to lead-based hybrid halide perovskites and is expected that the physical properties may be further enhanced by band gap tuning. We employ the Density functional theory to investigate the effect of the compressive and tensile strains on the electronic and optical properties of the $Cs_2AgInBr_6$. It is observed that the band gap changes about 7.55 (9.43) % under the 10% tensile (compressive) strain without changing the direct nature of band gap at Γ point in addition to higher hole mobilities under compressive strain due to high dispersive nature of Valence band maximum (VBM). The absorption peaks exhibit red shift by varying compressive to tensile strain however, reflectivity is almost flat in low energy region. Henceforth, the band gap tuning without affecting the direct nature of band gap with higher mobilities of both charge carriers along

with optical properties enhancement under the strain indicates potential photovoltaic material $Cs_2AgInBr_6$ with improved photo-conversion efficiency.

g0043

Strain Driven Electronic Topological Transition in Half Heusler LiCdAs: A Cubic Symmetry Breaking Approach

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The present work investigates the uniaxial strain induced Electronic Topological Transition (ETT) in Half-Heusler (HH) compound LiCdAs employing density functional theory. LiCdAs exhibits semi-metallic (SM) nature under normal condition, whereas, on breaking cubic symmetry at 2% uniaxial strain a spin-locked surface state is observed. The calculated Z_2 invariant predicts the non-trivial signature of LiCdAs. (i.e., $Z_2 = (1, 0\ 0\ 0)$). Such sensitive electronic properties under strain of LiCdAs makes it a suitable applicant for spintronics and nano-electronics applications.

g0044

Computational Modelling of Morphology Evolution in Multifunctional Tin-Oxide

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With the growing need to detect toxic gases in closed environments, functional and semiconducting metal oxide materials are being employed as gas sensors. In this paper, we report the effect of particle morphology on the sensing capabilities of tin-oxide (SnO_2) using molecular dynamics (MD) simulations. The results of MD simulations are used to model SnO_2 layers with different porosities, morphologies, dopants, and corresponding diffusion coefficients are calculated at room temperature. It is observed that, amongst different structures simulated in this work, the CNT decorated hollow nanostructures of SnO_2 show the highest diffusion coefficient (3982 $Å^2$/ps) for methane gas detection. Improved diffusion corresponds to a shorter response time, leading to faster signal generation and rapid methane gas detection.

g0045

Layer Dependent Semiconductor to Metal Transition in $PtSe_2$: From First Principle Calculation

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Platinum-based transition metal dichalcogenides (TMDs) have been gaining renewed interest due to their intriguing physical properties for both fundamental research and potential applications in electronics, optoelectronics and so on. Here, we investigate layer-dependent

tuneable electronic properties of platinum di-selenide ($PtSe_2$) by using only first principle calculation, *i.e*., density functional theory (DFT). First principle calculation predicts that the lattice constant increase with the increase in layer numbers along with the finding that the nature of mono- and bilayers are indirect semiconductors with band gaps of 1.42 eV and 0.43 eV, while few-layers and bulk counterparts shows metallic nature. From the energy band diagram, we observe the decrease in the indirect band gap values with increase in thickness due to quantum confinement and interlayer interaction. The aforementioned tuneable electronic properties make $PtSe_2$ a suitable candidate for the future nanoelectronics and optoelectronics applications.

g0046

Crystal Dynamics of Cu_3Au using pseudopotential theory

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In the present study, theory of pseudopotential has been used to calculate lattice dynamics of Cu_3Au alloy. For the evaluation of phonon frequencies (in symmetry & non-symmetry directions) and elastic constants, a recently proposed pseudopotential is employed which is determined using Generalized Pseudopotential Theory (GPT). Computed results are found to be in good agreement with available experimental results. The computed results justify the present pseudopotential's ability for transition metal's alloy.

g0047

First Principles Study on Structural and Electronic Properties of $CsPbI_{3-X}Br_X$ (X = 1, 2) Under Strain

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All inorganic cesium lead halide perovskites have gained extensive attention as promising photovoltaic materials for highly efficient solar cells. In this study, effect of strain on structural and electronic properties of $CsPbI_3$-xBr_X (X = 1,2) have been investigated using DFT-based first principles calculation. Both $CsPbI_2Br$ and $CsPbIBr_2$ have shown increasing of bandgaps with the applied strain. By introducing strain in the range of -3 to 3%, band gap of $CsPbI_2Br$ and $CsPbIBr_2$ have been tunned from 1.03 to 1.51 eV and 1.17 to 1.81 eV, respectively. Furthermore, the decomposition energy of $CsPbI_2Br$ and $CsPbIBr_2$ have been calculated to be -0.06 and -0.11 eV, respectively, demonstrating the higher stability of mixed halide cesium lead perovskites with more Br components. These findings will help researchers for better understanding the impact of strain on semiconductor material properties and for directing experiments to increase photovoltaic performance of cesium lead halide perovskites.

g0048

Ab-initio Simulations of Generalized Stacking Fault Energies in Cu.

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First principles simulations were performed to calculate the structural parameters and generalized stacking fault energy (GSFE) of Cu with two different PAW pseudopotentials. Our results show that the GSFEs are more sensitive to the type of the pseudopotential than to the number of layers used to simulate the system with stacking faults. The GSFE surface generated using the energy values was incorporated into a phase field dislocation dynamics (PFDD) model. The dissociation of screw dislocations into leading and trailing partials are shown using this multi-scale model, as a first step towards validation.

g0050
First Principles Insights of Dzyloshinkii-Moriya Interaction in TiI_3 Monolayer
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The first principles investigation of the structural and electronic properties of TiI_3 monolayer (ML) has been performed. TiI_3 ML has a triagonal structure with lattice parameter 7.25 A˚. The spin-polarized electronic properties propose TiI_3 ML as a ferromagnetic semiconductor. The hybridization of *p-d* orbital near the valence band maxima (VBM) and conduction band minima (CBM) can be observed, in both spin up and spin down cases. The feeble variations in the structural parameters, viz. bond length and bond angle, in presence of external electric field is evocative of weak Dzyloshinkii-Moriya interaction among nearest Ti spins, resulting in frail magnetoelectric effect within TiI_3 ML.

g0051
Ab-Initio Insights on the Electronic and Optical Properties of ZnS/CNT Core/Shell Nanowire
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Theoretical calculations of electronic and optical properties of ZnS/CNT(n,n) core/shell (c/s) nanowires (NWs) was carried out. It was observed that ZnS core with (9,9) chiral armchair carbon nanotube (CNT) is the most stable c/s configuration. Dirac metallic cones were observed in the band structures of CNT(9,9) and an indirect bandgap of 3 eV was observed in bare ZnS NW. The optical properties of ZnS/CNT(9,9) seemed to be a superposition of the bare counterparts, with high absorption in the ultraviolet (UV) and infrared (IR) regions.

g0052
Effect of Mn doping in Bi_2Se_3 topological insulator: probed by DFT and ARPES
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Magnetic ion doping in topological insulators has emerged out to be important both from technological point of view and for experimental verification of exotic fundamental physical concepts. Magnetic ion doping not only opens up the energy gap in surface states of a TI but also changes its bulk band structure significantly. To observe the effect of magnetic ion doping on electronic band structure of TIs we have performed high-resolution angle-resolved photoemission spectroscopy measurements and first principal DFT calculations on pure and Mn doped Bi_2Se_3.

g0053

Influence of Fe Doping on the Electronic Structure of Kagome Semimetal CoSn

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Electronic structure of Kagome semimetallic compounds $Co_{1-x}Fe_xSn$ (x=0, 0.2) studied using synchrotron photoemission and x-ray absorption spectroscopy. Compared to CoSn the Co 2p core-level peaks in $Co_{0.8}Fe_{0.2}Sn$ are found to be broader with reduced spin orbit splitting. The valence band of $Co_{0.8}Fe_{0.2}Sn$ also showed increased bandwidth of the d bands as compared to CoSn with prominent decrease in the intensity of the localized states near the Fermi level. The increased width of both the valence band and core level features in $Co_{0.8}Fe_{0.2}Sn$ indicates strong hybridization between Fe 3d and Co 3d states while decrease in the spin orbit splitting is related to the near neighbour electronic d-d interactions. We find that there is an interplay between the hybridization and electron-electron interaction in the Fe doped CoSn compound which influences the reported magnetic properties.

g0054

Spectroscopic and DFT based Computational Investigation of Nonlinear Optical Responses of Pyrrolidine derivative

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Organic materials have occupied new corners in the field of nonlinear optics (NLO). The organic NLO compounds are considered more efficient than the inorganic ones. The introduction of organic compounds having better NLO responses than the synthesized ones is an innovative idea to enhance the uses of organic compounds and bring subsequent advancement in the technology. The NLO materials are in high demand in the field of optical frequency conversion and generations, lasers, photonics, dynamic holography, telecommunications, etc. Thus, the introduction of such organic NLO agents give a wide area of research to young research aspirants. Therefore, we have considered the organic derivative of pyrrolidine for the present study. The NLO behavior of organic compound 1-(4-nitrophenyl)-2-pyrrolidinemethanol (NPM) has been successfully predicted by computational method using density functional theory with B3LYP/6-311G basis set. The

Mulliken charges and the molecular electrostatic potential is calculated for the prediction of the intramolecular charge transfer within the molecule. The values obtained for the frontier molecular orbitals and polarizability parameters validate the NLO responses of the molecule. The UV-Vis spectral analysis validates the electronic transitions within the molecule.

g0055

Multi-band slotted Microstrip Patch Antenna for S-band, C-band, X-band & Ku-band Applications

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A great antenna magnificent gave on account microstrip patch slotted antennas owing to their conciseness and incorporation in the field of communication. So as to refine gain and bandwidth, large-scale research is executed in the patch antennas. Several investigators have been communicated the systematic forms like circular, rectangular, and square patches. A novel design of six rectangular cuttings with a T-Slot patch antenna is considered and analyzed in this research article. To tune the characteristics and to enhance the outcomes of rectangular patch antenna (RPA) slot cutting techniques are used. Quint-bands are realized by introducing slots in the rectangular patch. It achieves five-band resonant frequencies having the highest gain of 15 dB, the radiation efficiency of 1.5815 at 14.79 GHz having the dimensions of 26 x33 x 1.6 mm. It is evident from the outcomes that gain became greater, the radiation efficiency is enhanced, return loss is minimized and quint band frequencies are achieved in a wide band range having the slots on patch antenna. The proposed construction makes the antenna reliable in design and facile for fabrication by enrolling slots in the patch. It covers the application of weather radar, surface ship radar, WiMAX (3.52 GHz), long-distance communication (7.72 GHz), satellite and space communication, terrestrial broadcast radar, amateur radio (11.50 GHz, 11.85 GHz), Satellite communication (14.79 GHz).

g0056

Thermal Effects on Mc-Si Ingot Growth Through Directional Solidification Process with Conventional and Modified Retorts: A Numerical Investigation

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In this paper, the results of the ingots grown with the conventional retort and modified retorts which are insulation inserted in bottom, center, and top of the retort respectively are compared with each other. The heat dissipation was analyzed by placing two thermocouples TC1 and TC2 near the side graphite heater and heat exchanger block respectively. By controlling the heat dissipation, the melt crystal interface could be maintained as convex or flat interface shape which is one of the key factors to grow good quality mc-Si ingot. The results shows that the ingot grown by the directional solidification furnace by modified retorts have more heat dissipation due to the insulation inserted in the retort as compared to the conventional retort.

g0057

Enhanced Optoelectronic Properties of 2D Hetero-bilayer HfS_2/GaS

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In the present study, the stability, electronic structure, and optical properties of the 2D van der Waals (vdW) have been systematically discussed within the framework of the Density Functional Theory (DFT). For the different stacking arrangements, the HfS2/GaS has exhibited the semiconducting characteristics with reduced electronic direct and indirect bandgaps. It has shown strong optical absorption in comparison to single-layers HfS2 and GaS. The enhanced optical and electronic properties of the HfS2/GaS suggest it as potential materials for applications in optoelectronics and nanodevices.

g0058
Exploring Topological Features in Chalcopyrite $ZnXBi_2$ (X = C, Si, Ge, Sn, and Pb)
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After the discovery of topology in materials, researchers are intensively searching for promising topological material candidates. We carried out a computational search for the topological features in the chalcopyrite family $ZnXBi_2$ (X = C, Si, Ge, Sn, Pb). We checked the stability of these materials at different hydrostatic pressure. These materials show thermodynamic stability at negative pressure. ZnSnBi2 is the least unstable material in the family and can be a good candidate for experimentalists to hunt for. We searched for the Weyl points and corresponding Chern numbers. The number of Weyl points and Chern number is found to be consistent with symmetry operations of the space group $I\bar{4}2d$.

g0059
Numerical Investigation on mc-Si Growth process by Directional Solidification for enhancing solar cell efficiency
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2D numerical simulation was carried out for growing high quality mc-Si ingot by directional solidification (DS) for enhancing performance of solar cells. The finite volume method is used for the discretization of DS system. The melt-crystal interface has a crucial role in controlling the impurities and dislocation generation in grown crystals. In this present work, the melt-crystal interfaces were studied for the different growth stages. Also, we have investigated the carbon (C) and oxygen (O) impurities.

g0060
Sodium Decorated Gallenane Layer for CO_2 Adsorption
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In this work, we investigate the results from the first-principles method based on the electronic structure calculations and study the adsorption properties of CO_2 molecule on gallenane (GaH) and sodium decorated gallenane (Na@GaH). The most stable configuration

for adsorption on Na@GaH is determined, and the structural parameters, adsorption energies and electronic structure are calculated. The adsorption energies of CO_2 on Na@GaH are significantly improved as compared to GaH and CO_2 is chemisorbed on Na@GaH. Our findings indicate that Na@GaH could be a promising candidate for molecule adsorption.

g0061

Electronic Structure Studies of Dihydrated 2,4,6-triaminopyrimidinium-3,5-dinitrobenzoate Proton Transfer Complex: A Comparative Analysis

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Herein, the electronic structure of the dihydrated proton transfer complex 2,4,6-triaminopyrimidinium-3,5-dinitrobenzoate has been compared with its constituents. Henceforth, molecular electrostatic potential mapping of the titled molecular complex along with its reactant molecules have been investigated thoroughly. Further, the effect of natural atomic charge rearrangement after complex formation has been examined critically by theoretical calculation at DFT/B3LYP/6-311++G(d,p) level of theory.

g0062

First Principles Study of Structural, Elastic & Electronic Properties of Hafnia Polymorphs

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Hafnium dioxide (HfO_2) is a technologically important material in the semiconductor industry. However, there is a limited literature on the elastic and electronic properties of all five polymorphs of HfO_2. We report structural, elastic and electronic properties of monoclinic, tetragonal, cubic and two orthorhombic phases of HfO_2 using Density Functional Theory (DFT) simulations and compare our results on structural and elastic properties with available experimental and other DFT results.

g0063

Spectroscopic Characterization and DFT Study of (E)-2-(1-(3-oxo-1,3-diphenylprop-1-en-2-yl) pyridin-2 (1H)-ylidene) Malononitrile

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Nonlinear optical (NLO) crystals having good stability, high transparency in the visible region and superior nonlinear susceptibilities are noteworthy due to their influence on the development of laser technology and optoelectronic industry. Theoretical study of nonlinear optical behaviour was done using B3-LYP/6-311G (d) basis set in Gaussian 09 program. The first hyperpolarizability of the molecule was computed by density functional theory. The observed vibrational wavenumbers in the experimental spectra were compared with the calculated results. From UV-vis absorption spectrum, excitation energy, maximum absorption wavelength and optical energy band gap have been performed. The HOMO-LUMO energy gap of the compound is calculated. HOMO and LUMO energies reveal the chemical reactivity, kinetic stability and hardness of molecule.

g0064

Structural and Electronic Properties of α-Ca_3N_2 :A First Principles Study

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In this paper, we investigated the structure and electronic properties of α- Ca_3N_2 compound using the first principles linear combination of atomic orbital (LCAO) method. Structural properties are determined by optimizing the experimental structural parameter under DFT-GGA framework. The electronic properties of optimized structure show semiconducting nature of α-Ca_3N_2. The energy band gap of α-Ca_3N_2 lies within the range of optimum energy of solar spectrum, hence making it suitable candidate for photovoltaic applications.

g0065

Electronic And Elastic Properties Of CeX (X = Cd &Hg) Intermetallics: An Ab-Initio Study

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An ab-initio calculations have been performed to investigate the electronic and elastic properties of CeCd and CeHg intermetallics using density functional theory. The electronic properties have been studied throughout the calculations of the band structure and charge density distributions. From band structure calculations, it is revealed that both the intermetallics exhibit metallic character. The ductility or brittleness of these compounds is predicted from Pugh's rule (B/G_H) ratio.

g0066

Thermodynamic Properties of Pure and Li Adsorbed Graphene from Vibrational Modes

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Various thermodynamic properties of pure and lithium-adsorbed graphene ($Li@G_{32}$) are calculated using their phonon dispersion curves. The phonons are calculated using Ab initio density functional perturbation theory (DFPT). The phonon dispersion curves show significant change at low frequencies on Li adsorption. The density of states (DOS) reflects the presence of Li atom and the specific heat, entropy and free energy of these two systems have been plotted as a function of temperature.

g0067

Photoemission Spectroscopy of $ACu_3Ru_4O_{12}$ (A = Ca/La)

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We investigate the electronic structure of *A*-site ordered cubic perovskites $ACu_3Ru_4O_{12}$ (*A* = Ca/La) using *x*-ray photoemission spectroscopy and *ab-initio* band structure calculations. Valence band spectra exhibit large intensity at Fermi level, E_F, for $CaCu_3Ru_4O_{12}$ and $LaCu_3Ru_4O_{12}$ commensurate with highly metallic character of these systems. Band structure calculations within local density approximation (LDA) fail to capture the position of Cu 3*d* derived features, while all the features are well reproduced by inclusion of strong correlation for Cu 3*d* electrons within LDA+U ($U_{Cu\ 3d}$ = 4 eV). While the delocalized Ru 4*d* states hybridize strongly with O 2*p* states, the Cu 3*d* states are essentially localized and appear above 2 eV binding energy. Observation of larger intensity of O 2*p* spectral features in the valence band spectrum of $LaCu_3Ru_4O_{12}$ than that of $CaCu_3Ru_4O_{12}$ may be related to larger La - O hybridization in $LaCu_3Ru_4O_{12}$.

g0068

Dynamical Studies for bcc Niobium

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In this study, we proposed a transition metal pseudopotential (TMPP) and demonstrated its credibility by carrying out lattice dynamical studies for bcc Niobium (Nb). The generalized pseudopotential theory (GPT) is used to derive our proposed pseudopotential. We have calculated the values of phonon dispersion curves, dynamical elastic constants in long-wavelength limit ($\vec{q} \to 0$) and bulk modulus using this potential. In comparison to experimental data and other theoretical approach our results are quite encouraging.

g0069

Electron Correlation in (Ca/Sr)Pd_3O_4

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We investigate the role of electron correlation in narrow bandgap semiconducting ternary palladates (Ca/Sr)Pd_3O_4 using valence band *x*-ray photoemission spectroscopy and *ab-initio* band structure calculations. Experimental valence band spectrum exhibits negligible intensity at Fermi level, E_F. Overall description of the experimental spectrum is well captured in band structure calculation within local density approximation (LDA) but leads to a metallic ground state in contrast to semiconducting behavior. Electron correlation is included within LDA+U framework, which leads to opening of a gap at E_F for U > 4 eV. LDA+U (U = 4.5 eV) calculations exhibit direct bandgap at point with bandgaps of 0.062 eV and 0.049 eV for *$CaPd_3O_4$ and $SrPd_3O_4$, respectively*

g0070

Molecular Dynamics Simulations of Evolution of Radiation-Induced Defects in Nickel due to Low Energy Self-Ions

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The ion-induced primary radiation damage phenomena in pure nickel are investigated by simulating the evolution of cascade of 2, 5 and 10 keV Ni PKAs using molecular dynamics technique. The damage formation stabilizes after about 10, 15 and 18 ps for the 2, 5 and 10 keV PKAs, respectively. Large size clusters of point defects form as the system progresses towards the heat spike phase and after the system has evolved sufficiently, the interstitial clusters tend to remain in larger sizes as compared to the vacancy clusters. The formation of defects, especially in the form of large number of small clusters induce an average volumetric strain in the material which initiate around the local heat spike region. The system evolves to a state where defect formation has saturated and there is a reduced remnant average volumetric strain accounted to the existing stable point defects and larger clusters.

g0071
Analytical Approximation for Neutron Thermal Scattering Law with a Novel Form for Phonon Density of States
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Evaluation of Neutron Thermal Scattering Law S(α,β) is quite involved as the integrand has Fourier transform in the exponent which has no closed form expression. Computation of S(α, β) requires many approximations and extensive numerical calculations. We propose a novel form for the Phonon Density of States which gives closed form expressions for Fourier transform and leads to analytical approximations for S(α,β) making its evaluation far easier. These new approximations obtained are compared with values for example cases for BeO available in the literature.

g0073
Proposing And Modelling Chalcogenide Prism Model with Hyperbolic Metamaterials for Surface Plasmon Resonance Based Biosensing Applications
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A conventional biosensor detects higher molecular weight biomolecules quiet easily but detecting lower molecular weight biomolecules is a challenging task. We intend to over come this difficulty by proposing prism coupled Surface Plasmon Resonance (SPR) biosensor model that detects the lower molecular weighted biomolecules. In our proposed model, we have considered a chalcogenide prism with metal-dielectric (HMMs) multilayers and an analyte stacked over the prism in the krestchmann surface plasmon resonance (SPR) configuration and analysed the performance of the sensor metal-dielectric (HMMs) multilayers. Graphene and silicon carbide (SiC) is considered as one of the (HMMs) multilayer and the sensitivity of graphene-SiC (HMMs) multilayer structure based biosensor is determined by trans fer matrix approach.

g0074
Fermiology of Topological States in the Chiral Crystal RhSn

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Chiral crystals with well-defined handedness feature chiral massless excitations at the time-reversal-invariant-momentum (TRIM) points in the Brillouin zone. Here based on first-principles theoretical modeling, we discuss the role of crystal chirality in driving the chiral fermions in the momentum space in RhSn. We show that RhSn hosts multifold chiral fermions with associated surface Fermi arcs states that span the whole surface Brillouin zone. We also discuss the multiple topological gap structure and associated surface states in RhSn. Our study unfolds RhSn as a new Kramers-Weyl fermions semimetal with exceptionally long Fermi arc states that would be ideal for fundamental science and device applications.

g0077

Structural, elastic and anisotropic properties of Fe_2Zr and $FeZr_2$ intermetallics

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Fe-Zr based alloys, *viz.*, SS-15 wt% Zr and Zr-8 wt% SS are found to be promising materials for high level nuclear metallic wasteform. It has been observed that Fe_2Zr and $FeZr_2$ intermetallics appear dominantly in these alloys and act as a host for the radionuclides present in the waste. In this work, we have studied the thermodynamic, elastic and anisotropic properties of the Fe_2Zr and $FeZr_2$ intermetallics. It has been found that both the phases are thermodynamically as well as mechanically stable. The bulk (B), shear (G) and Young's moduli (Y) of Fe_2Zr phase are higher than that of the $FeZr_2$ phase. Both the phases are found to be ductile in nature. The anisotropic properties show that $FeZr_2$ phase is more anisotropic than the Fe_2Zr phase.

g0078

Electronic and optical response of twisted $MoS_2/MoSe_2$ heterostructure

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In recent time, twistronic is a center of attraction in the field of research for tuning and enhancing the physical properties of 2D bilayer and hetero-structures. In the present work, First-principles based Density Functional Theory (DFT) was used to investigate the opto-electronic properties of twisted $MoS_2/MoSe_2$ hetero-structure. Optical response shows that the twisted hetero-structures exhibit highest optical absorption in the visible regions. With varying the twist angle between the layers of hetero-structure, they make transitions between direct and indirect band gap semiconductors. These properties make the twisted hetero-structure as a promising candidate for application in next-generation Nano and optoelectronic device.

g0079

A Theoretical Study of the Electronic and Magnetic Structure of $Nite_2$

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Topological materials with protected electronic states hold promise for rich physics and various applications in spintronics. We investigate electronic topological property of type II Dirac semimetal $NiTe_2$ in which Lorentz invariance is broken. $NiTe_2$ exhibit type 2 Dirac fermions near the Fermi level. Our calculations show titled Dirac cones along along Γ-A high symmetry points. The metallic density of states (DOS) and the dominating contribution of Ni-3*d* and Te-5*p* orbital to the band structure is noticeable. This d-p hybridization allows the dirac point to exist close to Fermi energy.

g0080

Charge Transfer Mediated Hydrogen Evolution Reaction Over Co Loaded g-C_3N_4

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Highly photoactive transition metal decorated graphitic carbon nitride (g-C_3N_4) possess greater visible spectra absorption and large photo-generated charge separation attributing to formation of intermediate in narrowed forbidden region. Site dependent study of hydrogen evolution reaction (HER) using adsorption of H-molecule along with water molecule and role of charge transfer mechanism are reported for Co decorated g-C_3N_4 (Co-C_3N_4) using density functional theory. Adsorption of water molecule with H-atom over bay-Carbon (C_b) atom in Co-C_3N_4 shows 5.6, 7.3 and 4.6 fold decrease in overpotential than pristine g-C_3N_4, H-atom adsorbed at C_b and H-atom adsorbed at corner-Carbon (C_c) atom, respectively. Significant change in potential barrier is attributed to π-delocalization and charge transfer among H-atom and the C atom of Co-C_3N_4 for enhanced photocatalytic activity.

g0081

Impact of Spin-Orbit Coupling on the Electronic states of Ir ions in Rare Earth Double Perovskites Nd_2ZnIrO_6

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First Principle Study on Rare earth double perovskite Nd_2ZnIrO_6 gives antiferromagnetic arrangement within Nd and Ir ions as the ground state for the system. With the application of spin-orbit interaction, the Ir d states split up into jeff = 3/2 and jeff = 1/2 states and open up a small gap at the Fermi level and make the system a candidate for j_{eff} =½ mott insulator.

g0082

Effect Of ZnO Electron Affinity on Organic-Inorganic CH3NH3PbI3 Perovskite Solar Cell

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In this work, a Lead-based perovskite solar cell $CH_3NH_3PbI_3$ was simulated using the solar cell capacitance simulator. Theoretical validation of experimental results in perovskite solar cells with efficiencies of 27.53% is presented. The simulation effort is focused on the adjustment of the electron affinity of the electron transport material (ZnO) on photovoltaic properties of solar cell devices. Here we found a spike which acts as a barrier potential in the transportation of electrons from perovskite active layer to ZnO electron transport material by optimization of value of electron affinity to 4.0 eV and reducing this spike we got the efficiency of perovskite solar cell above 27.53%.

h: SINGLE CRYSTALS GROWTH AND CHARACTERIZATION

h0002

Investigations into Heme Detoxification Protein of Malaria Parasite

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Malaria remains the world's most prevalent human parasitic disease, claiming 1 to 3 million lives annually. Sequestration of cytotoxic free heme into inert hemozoin (Hz), is a bottleneck in the physiology of malaria parasites. "Heme detoxification protein" (HDP) has emerged as a prominent mediator for this process of detoxification. This process characterized by phase transformation of amorphous heme into crystalline Hz. Despite the importance, the mechanistic insight behind the functionality of HDP is yet to be revealed. Partly, the culprit for this lapse of information is the inability to produce recombinant native HDP. For the first time, we have purified a native fusion protein of HDP in complex with GroEL chaperonin. The crystals of this complex were diffracted on the PX-BL21 beamline at the Indus-2 synchrotron. The data was collected at 3.5Å resolution and processed in the P121 space group with unit cell dimensions of 283.48 Å, 135.53 Å, 283.62 Å, 90.00° 117.51° 90.00° [a, b, c (Å), α,β,γ, (°)]. The asymmetric unit has 28 chains (1,605.2 kDa) of GroEL, but we could not trace any chain for HDP fusion protein. By far, this is the largest structure ever been solved at PX-BL21 protein crystallography beamline. The final model has been refined to R_{free} of 26%.

h0003

Growth and Characterization of 2-Ethylimidazolium D(-) tartrate Crystal

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Single crystals of 2-ethylimidazolium d-tartrate ($C_9N_2O_6H_{14}$) were grown by slow evaporation solution growth technique at ambient temperature in deionised water as solvent. The grown crystals were characterized by single crystal XRD using MoKα (λ=0.71073Å) radiation and the lattice parameters have been obtained. The Fourier Transform Infrared Spectroscopy of 2-ethylimidazolium d-tartrate reveals the presence of ethyl and carboxyl functional groups in the compound. The optical transparency window in the UV-Vis region is found to be good for nonlinear optical applications. The TGA and DTA reveal that the title compound incipient melting occurs at 148.34°C. The theoretical factor group analysis predicts 372 optical modes in the grown title compound. The SHG behavior of the title compound was demonstrated using Q-switched Nd: YAG laser.

h0004

Crystallization Of Insecticidal Toxin, Txp40 From*Xenorhabdus nematophila.*

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Txp40 is 42 kDa potential and ubiquitous toxin from *Xenorhabdus* and *Photorhabdus* bacteria, it is active against wide range of insect pests. Txp40 shares no significant structural

match to proteins with known structures or functions, which suggests that it is a novel protein. Here, crystallization and preliminary x-ray analysis of Txp40 toxin from *Xenorhabdus nematophila* (ATCC 19061) is reported. Purified Txp40 was crystallized using under oil microbatch technique. Single crystal X-ray diffraction data was collected on the PX-BL21 beamline at the Indian synchrotron to 2.2 Å resolution with 100% completeness. Crystal belongs to $I2_12_12_1$ space group with unit-cell parameters a = 94.44, b = 97.62, c = 148.97 Å, Calculated Matthews coefficient was 2.06 $Å^3$ Da^{-1}, with a corresponding solvent content of 41%. Structural analysis of Txp40 will provide new insights about mode of action of this toxin and because of its novel status it is highly possible that crystal structure of this protein will introduce a new domain and/or motif in the area of insect toxicity.

h0005

Crystal Growth, Structural and Optical Characterizations of 1,2,3- Benzotriazole 2-chloro-4-nitrobenzoic Acid (BCNB) Single Crystal for Nonlinear Optical Applications

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The third order nonlinear optical organic single crystal of 1,2,3- benzotriazole 2-chloro-4-nitrobenzoic acid (BCNB) was grown by slow evaporation solution technique (SEST) using methanol as the solvent. The lattice parameters of the grown crystal were confirmed by single crystal X-ray diffraction (SXRD) analysis. It shows that BCNB single crystal belongs to the monoclinic crystal system with the space group P21/n. UV-Vis-NIR analysis shows that the grown crystal has good optical transmittance in the entire visible region. The grown crystal was subjected to the photoluminescence (PL) and the emission peaks were obtained at 363 nm and 448 nm. The laser damage threshold (LDT) value of BCNB was found to be 13.8 GW/cm2.

h0006

Single Crystal Growth, Electrical, and Magnetic Properties Studies on Hexagonal $Co_{0.82}Se$

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We successfully have grown high quality single crystals of $Co_{0.82}Se$ by flux-free melt growth process. Structural and elemental analysis have been performed using X-ray diffraction (XRD) and energy dispersive X-ray spectroscopy (EDXS), respectively. The XRD patterns confirm hexagonal crystal structure of the compound with a $P6_3/mmc$ space group. We have measured electrical resistivity of $Co_{0.82}Se$ within the temperature range of 2-300 K. From the Bloch-Grűneisen (BG) fitting of the resistivity data suggest for a dominant electron-phonon scattering in this system with a Debye temperature of 254 K. Magnetization measurements suggest that these are paramagnetic systems in nature.

h0007

Antielectrostatic Hydrogen Bonding between oxyanions and their tendency to form proton wires within crystals: A Cambridge Structural Database Study

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Cambridge Structural database (CSD) was searched for salt crystals containing oxyanions HSO_4^{1-}, $HSeO_4^{1-}$, $H_2PO_4^{1-}$,$H_2AsO_4^{1-}$, NO_3^{1-}, ClO_4^{1-}, and it was found that all these ions with an exception of ClO_4^{1-} have a tendency to make strong Antielectrostatic hydrogen bonds (AEHB) between themselves, many of these salt crystal have extended networks of AEHBs which have the potential to act like proton wires allowing fast transport of proton within the crystals. Hence these crystals can be candidates for a technological important class of materials called Proton conductors. Likely Proton conduction pathway for one such crystal namely Pyrazinium hydrogen sulphate is compared to that found in well established proton conductor crystal $CsHSO_4$.

h0008

The croconic acid glycine crystallization and decomposition

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In an attempt to form new class of complexes of organic ferroelectric, it was decided to complex the organic ferroelectric croconic acid with glycine. The crystallization resulted in complex, ammonia oxonium di oxalic acid oxalate hydrate. It is seen that both croconic acid and glycine have undergone oxidation to oxalate and ammonia. The oxidation of croconic acid may be due to exposure to light, even though extreme care was taken to avoid light exposure. The oxidation of glycine though seen in animals and humans in the presence of enzyme, here it occurs due to croconic acid.

h0009

Structural and Spectroscopic Study on Ytterbium Tri Chloride($YbCl_3$)

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The crystals of $YbCl_3$ were grown by the slow evaporation technique and characterised by scanning electron microscopy, x-ray diffraction, uv-vis, fourier transform infrared spectroscopy and photoluminescence. The crystal is crystallized in monoclinic structure. The energy gap is deduced as 4.41 eV which confirms the insulating nature and Urbach energy is 0.6567 eV. Photoluminescence study showed the presence of Ytterbium vacancy-related defects.

h0010

Growth of $Cd_{0.90}Mn_{0.10}Te$ Single Crystal by Vertical Bridgman-StockbargerMethod

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CdMnTe (CMT) is a cadmium telluride-based compound semiconductor crystal for application in room temperature radiation detection. This material attracts interest to replace

CdZnTe (CZT) because of its uniform segregation co-efficient of Mn, high resistance and tunable bandgap of the crystal. This manuscriptreports the growth and structural characteristics of the grown crystal. In this work the $Cd_{0.90}Mn_{0.10}Te$ single crystal was grown by vertical Bridgman-Stockbarger method. The grown single crystal was characterized by powder X- ray diffraction, Laue diffraction, NIR and Fourier TransformInfra-Redspectroscopy.

h0011

Single Crystal Growth Of $LiCoO_2$ Using Optical Floating Zone Technique

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High purity, phase pure single crystals of $LiCoO_2$, with various excess Li concentration (8% and 12%), and no excess Li, were grown using the optical floating zone furnace. The single crystals of $LiCoO_2$ have been known for their potential applications as an active cathode material in rechargeable Li-ion batteriesThe rigorous experiments and observations conclude that the phase pure single crystals of $LiCoO_2$ can only be grown by optimizing the parameters governing the stability of the molten zone i.e. the crystals are grown in the Argon atmosphere with a pressure of 8.5 bar, with growth speeds of 1.0-2.5 mm/h, using no excess Li concentration. The Laue diffraction studies confirms the crystal structure to be Rhombohedral with space group $R\bar{3}m$. The dc magnetization studies of the grown crystal show a metal-insulator transition at around 270K and a short-range magnetic ordering at 110K. The $LiCoO_2$ single crystal shows no hysteresis even at higher temperatures.

h0012

Thermal Investigation Of $CuFeS_2$ Single Crystals

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The thermal behaviour of $CuFeS_2$single crystalsgrown by chemical vapour transport technique are discussed in this paper. The thermogravimetric, differential thermogravimetric and differential thermal analysis curves of the grown crystals are measured between ambient and1203 K temperatures. The thermocurves are measured in argon atmosphere for three heating rates of 10, 15 and 20 $K \cdot min^{-1}$. The kinetic parameters are evaluated employing three different relations and obtained kinetic parameters are discussed.

h0013

Seebeck Coefficient of Ni doped Bi_2Te_3

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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. Which results in the suppression of carrier mobility and electrical resistivity reducing the Seebeck coefficient with increasing doping concentration.

h0014

Optical and Laser Characteristics of Nd doped $LuVO_4$ Single Crystal Grown by OFZ Method

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Single crystals of Nd (0.5 at.%) doped $LuVO_4$ were grown by optical floating zone technique. The strong absorption band of Nd:$LuVO_4$ crystal centered at 810 nm can be used for efficient pumping to the Nd:$LuVO_4$ laser gain medium by using a diode laser operating ~ 810 nm wavelength. The PL intensity at 1065 nm was the highest for both excitation wavelength at 810 and 880 nm. CW Laser emission at 1066 nm was demonstrated and the output power for Nd:$LuVO_4$ element 360 mW.

h0015

Influence of Thermal Field on the Reduction of Stress and Dislocation Density in the Growth of mc-Si in DS Process

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Global modelling and transient simulation have been carried out on bulk multi-crystalline silicon (mc-Si) growth in an industrial directional solidification furnace. Modification on the heaters has been made to understand its influence over the thermal stress and dislocation densities. The uniform temperature distribution was achieved. The simulation confirms that the stress and dislocation density is decreased by controlling the thermal field of the furnace. The results show that, the influence of the temperature distribution can enhance the quality of the ingot which can be used to produce high efficiency photovoltaic cells.

h0016

In-house Development and Demonstration of Low Energy Gamma-ray Spectrometer Based on CdZnTe Single Crystals

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$Cd_{0.9}Zn_{0.1}Te$ (CdZnTe), single crystals were grown by the traveling heater method (THM). The crystal growth parameters, including growth rate, ampoule rotation, temperature profile, Te solvent and growth temperature were optimized to yield large-grained CdZnTe. The CdZnTe wafers were characterized for its structural and electrical properties. Fabricated CdZnTe detector with planar gold electrode was tested using a ^{241}Am source. The spectrum was acquired for 511 s at a bias voltage of 350 V with a shaping time of 0.5 μs. Photo peak

of ^{241}Am at 59.6 keV is well resolved. The energy resolution of this detector was found to be 8.46 % at 59.6 keV.

h0017

Investigation of Pyroelectric Energy Harvesting Potential of $LiTaO_3$ Single Crystal

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Pyroelectric energy harvesting is gaining attention for harnessing waste thermal energy into useful energy. We are reporting pyroelectric energy harvesting studies performed on $LiTaO_3$(LT) crystal wafer using an in-house developed experimental set up. Setup consists of a thermoelectric Peltier heating module and LABVIEW based electronic control circuit & data login interface. [001] oriented wafers of 15mm dia. and 0.7mm thickness were fabricated from the grown crystal. Experiments were performed for different heating/cooling rates. The heating/cooling cycle of LT wafer from 30 to 45°C generated a peak voltage ~25μV for ΔT~15 °C, which depicts the energy harvesting potential of LT crystals.

h0019

Growth of High Quality Single Crystals of Bi_2Se_3 Topological Insulator via Vertical Bridgman Technique

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Topological insulators (TI) are the new state of quantum matter with unique surface properties which has several applications inthe field of spintronics and other modern technologies. Device applications require a very good quality sample. Till now people have tried several methods for designing TIs. Here, we used vertical Bridgman technique for growing good quality single crystals of pure and Mn doped Bi_2Se_3. X-Ray diffraction has been performed to confirm single phase and Hall measurement done for studying the electronic properties of Bi_2Se_3 and Mn doped Bi_2Se_3 single crystals. It is observed that Mn in Bi_2Se_3 decreases the mobility of charge carrier which explained in terms of crystal defects which produces due to charge compensation. And also Hall coefficient is found increasing due to Mn doping.

h0020

Synthesis and Structural Characterization of Methylammonium Lead Bromide Single Crystal, Grown by ITC Method

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Bulk single crystals of a Lead halide perovskites perform better than the corresponding polycrystalline samples in many applications and hence, the preparation of large-sized as well as high-quality single crystals is necessary to enhance the device performances. In the present study, Methylammonium lead bromide single crystals are synthesized with a slight

modification in the well-known inverse temperature crystallization method reported in literature. The structural characterization of the synthesized single crystals was performed using synchrotron x-ray diffraction technique. Peaks corresponding to only a particular set of planes were observed confirming the formation of single crystal. Powder diffraction was also performed on the same sample to check for the phase purity of the prepared sample.

h0021

Synthesis and Optical Characterization of $Bi_{1-x}Z_xO$ (x=0.15) Thin Film

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Bismuth Zinc Oxide(BZO) is a potential material for different application due to its small bandgap(~2.92eV) and shows high-efficiency photocatalytic activity. The adopted method (modified Sol Gel) is a cost-effective method in comparison to the available methods like solid-state reaction, traditional sol-gel method, wet chemical method etc. The optical parameters like band gap, dielectric constant, transition strength, energy loss function are estimated for the film and observed to be a suitable candidateforindustrialapplicationsinphotovoltaic.

h0022

Growth and Characterization 2AP4N Single Crystal by Immersing Ampoule Sankaranarayanan–Ramasamy (ISR) Method

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The optically good quality organic 2-aminopyridinium 4-nitrophenolate 4-nitrophenol (2AP4N) single crystal of length 120 mm and diameter 15 mm was grown by a novel Immersing ampoule Sankaranarayanan–Ramasamy (ISR) method. The water covered completely the glass ampoule containing growth solution in the unidirectional method for the first time in the literature. The ampoule was specially designed for the growth of good quality and bulk size unidirectional single crystals by slow cooling condition. The unwanted temperature gradient developed on the solution surface was completely avoided and hence the secondary nucleation developed on top of the glass ampoule is avoided. The growth apparatus and optimization parameters have been made simpler compared to the conventional SR method. The optical behavior of the grown 2AP4N crystal was analyzed by UV-Vis NIR spectrophotometer. The optical homogeneities of the grown 2AP4N crystal were analyzed by birefringence measurement. The growth of <001> direction was confirmed by the PXRD analysis. The crystalline perfection of different growth portions (bottom, middle and top) was confirmed and analyzed by HRXRD measurement. The various studies reveal that the ISR method grown single crystals are favorable for high performance optical device applications.

h0024

Evidence of Cubic Structure and Topological Crystalline Behavior of SnTe at Low Temperatures

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We investigate the growth of high quality single crystalline SnTe, a rare topological crystalline insulator and its topological property employing angle resolved photoemission spectroscopy (ARPES). The outstanding problem in SnTe is the transition from highly symmetric cubic phase to a relatively lower symmetric rhombohedral structure at low temperature which is less favorable for topological behavior. We have grown high quality single crystals of SnTe using modified Bridgman method. The structure analysis reveals cubic structure down to 2 K studied. ARPES results are found to be consistent with the band structure results. The data collected at low temperatures show Dirac cone, a characteristic of the topological behavior. These results suggest that the cubic structure is the ground property of SnTe and that the structural distortion observed in earlier studies maybe linked to the Sn-vacancy.

h0025

Directional growth, Structural and Optical Properties of 2-Amino-5-Nitropyridinium p-Toluenesulfonate (2A5NPT) Single Crystal for Nonlinear Optical (NLO) Applications

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An efficient organic NLO single crystal of 2A5NPT was successfully grown by the modified SR method with a span of 60 days. The formation of the title crystal and its crystalline perfection were evaluated by SXRD and HRXRD analyses, respectively. The modified SR method grown crystal possesses 82% of optical transmittance in the visible and NIR region. The third-order NLO response of the grown crystal was determined by the single beam Z-scan technique using He-Ne laser of wavelength 632.8 nm. The obtained results evidence that the title crystal has the behavior of negative nonlinear refraction and reverse saturable absorption.

h0026

Single Crystal Growth Of Calcium Based Transition Metal Pnictides Ca*TX* (*T* = Au, Ag, Cu and *X* = Bi, Sb, As) and Their Transport Properties

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Calcium base transition metal pnictides materials are interesting to their inherent electronic band structure. Here, we report detail single crystal growth techniques of CaAuAs, CaAgAs, CaAgBi and CaCuSb. All the mentioned materials are grown by flux method. All specified flux compositions and temperature profiles are mentioned for grow single crystals. Temperature dependent resistivity of these materials show a metallic nature. For CaAgBi and CaCuSb, the magnetoresistances (MRs) show a cusp like behavior, whereas this behavior is absent for CaAgAs and CaAuAs. This cusp like feature is reminiscent of weak antilocalization where the quantum interference plays a crucial role. MR in CaAgAs and CaAuAs are almost linear.

h0027

Growth of Halide Scintillator Single Crystals Using Multi-Ampoule Bridgman Technique

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A multi ampoule Bridgman technique for growth of halide single crystal is developed, which enables growth of 4 single crystals simultaneously in single experiments and it helps for precise comparison in crystals without compromising in crystal quality. The scintillation performance of grown crystals are compared with standard data which is available in literature and found that there is no significant change in energy resolution. Multi ampoule Bridgman technique found to be very economical for research purpose.

h0028

Role of Nitrogen Incorporation in Growth of Large Area Homo-epitaxial Single Crystal Diamond

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Due to the wide range of exceptional properties, diamonds have become a most promising candidate in the field of electronic and optical applications. High-density microwave plasma chemical vapor deposition technique was employed to grow a high-quality single-crystal homoepitaxial diamond films. It has been shown that the phase purity, surface morphology, and growth rate of deposited diamond increase by feeding a small concentration of nitrogen to the gases phase. Freestanding homoepitaxially synthesized specimens have been characterized using Raman Spectroscopy, XRD, and Atomic forced microscopy (AFM). An intense Raman peak at about 1332.8 cm^{-1} confirms the Single phonon Brillouin zone centre corresponds to the Single crystal diamond.The surface morphology of grown samples using AFM measurement reveals that the sample with a high concentration of nitrogen (~ 9 ppm) gives a better result.

h0029

Third order nonlinearity of Ethyl p-amino benzoate (EPAB) single crystal grown by Solution and Bridgman technique – A Comparative Analysis

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Single crystals of Ehtyl p-amino benzoate has been grown by solution growth and Bridgman technique. A comparative analysis about the growth and optical properties of the grown crystals were carried out. It was found that the EPAB crystal grown from Bridgman technique is having a high value of third order nonlinear susceptibility when compared with the crystals grown by solution growth technique.

h0030

3-(THIOPHEN-2-YL)-5-(4-(TRIFLUOROMETHYL)PHENYL)-4,5-DIHYDRO-1H-PYRAZOLE-1-CARBOXAMIDE

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Title compound was synthesized, and its crystal structure was investigated by X-ray crystallography. Title compound was synthesized, and its crystal structure was investigated by X-ray crystallography. The molecule belongs to the monoclinic system. The space group is C2/c. The lattice parameters are a = 32.999(2) Å, b = 9.7141(5) Å, c = 20.8477(12) Å and β = 106.160(6)°. The final residual value is R1 = 0.1178.The molecule exhibits both intermolecular and intramolecular N−H...S, C−H...S and N−H...N, C−H...N hydrogen bonds.

h0031

Development of SEM Detectors using IndigenousYAP:CeScintillators

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Scanning Electron Microscope (SEM)is a significant micro-imaging and characterization tool that has gained popularity among all disciplines of science. Bhabha Atomic Research Centre, Mumbai has been involved in indigenous development of SEM to make the technology affordable for Indian academia and to cater to special requirements of the department. Here we discuss about design and development of indigenous SEM detectors using in-house developed YAP:Ce scintillators.

h0033

Multriticality in Quasi-kagomeFerromagnetURhSn

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We report high quality single crystal growth of ferromagnetURhSn, crystallizing in ZrNiAl-type hexagonal structure in which the magnetic U-atoms form potentially frustrated quasi-kagome two-dimensional net. Our measurements of electrical transport under hydrostatic pressures up to 11 GPa reveals two bicritical points concurrent at P_C = 6.25 GPa corresponding to its successive double phase transitions (T_O = 54K, T_C = 18K at ambient). Rermakably, the intermediate phase remains hidden as local probes like neutron scattering and Mossbauer spectra do not capture any new feature between the TC and TO. Our low temperature resistivity data under pressure points out a Fermi surface reconstruction across the PC, corresponding to an unconventional class of quantum phase transition involving multicritical points. This picture is further ascertained by gradual development of $-\ln T$behavior in 5f-derived electrical resistivity and appearance of T5/3 behaviour in the pressure induced phase.

h0034

Reflux deposited ZnO Nanoparticles For Supercapacitor Application

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In the present work, zinc oxide (ZnO) nanocrystals have been prepared by the reflux method. Their structural, morphological, optical and capacitive properties have been investigated. Structural characterization by X-ray diffraction reveals that polycrystalline nature. Integration of ZnO was confirmed from elemental analysis using EDX. SEM technique proved that the successfully coated the surfaces of the nanostructures. The as-optimized binder-free ZnO nanoparticle electrode exhibited a reversible electrochemical feature, providing a high specific capacitance of 335 F g^{-1} at 5 mV $s^{-1.}$ These performances of ZnO nanoparticle were attributed to its open mesoporous and large accessible area of hierarchical nanocrystals.

i: TRANSPORT PROPERTIES

i0001

Dissipative Quantum Transport In Single Molecular Transistor At Finite Temperature And Magnetic Field: A Tunable Spin-filter

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The effect of magnetic field and temperature on the quantum transport is investigated in a single molecular transistor where a quantum dot containing a single-quantized energy level is inserted in the center and coupled to the source and drain. This three-terminal device is mounted on an insulating substrate which plays the role of a phonon reservoir. The dotconsists of an onsite electron-electron correlation, polaronic (electron-phonon) interaction and the coupling between quantum dot local phonon and the substrate phonon produces a quantum dissipative effect on the dynamics of conducting electrons. At first, the dot-substrate phonon interaction is eliminated by a canonical transformation. Then, the electron-phonon coupling is removed by a coherent-state phonon averaging via Lang-Firsov transformation under the framework of Anderson-Holstein-Caldeira-Leggett model followed by a mean-field Hartree-Focktechnique to treat the onsite Coulomb correlation. Finally, we calculate transport properties such as spectral density function, tunneling current, differential conductance and spin polarization employing finite-temperature Keldysh non-equilibrium Green function method to see the out-turn of temperature and an external magnetic field in the presence of damping, electron-phonon interaction and Coulomb correlation. It is shown that temperature has an intervening effect on the spin-resolved transport properties which can be used as a tunable spin-filter.

i0003

Dynamics of Liquid Gallium-A Microscopic Approach

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The modified microscopic theory has been used to study the collective dynamics of liquid Gallium for the wave vectors close to its melting point. The obtained energy dependent spectra for the dynamical structure factor of the liquid Ga sample are very much in accordance with the experimental values of coherent inelastic X-ray scattering

i0005

Enhanced Electrical Transport Properties of Ex-situ Ball-milled Silver Doped Hydroxyapatite for Rectifying Applications

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Silver-doped hydroxyapatite (Ag-H) synthesized by the hydrothermal method has been wet-milled for 30min (Ag-HM) and the structural, compositional and morphological characteristics have been compared before and after milling. Ag-HM shows improved ionic conductivity, significantly high dielectric permittivity, and less energy consumption at high

temperatures than that of Ag-H without any adverse change in its compositions and stoichiometry. Nonlinear back-to-back Schottky diode-type rectifying behavior for high temperature regime(373-613 K)has been reported for the first time for milled silver-doped hydroxyapatite.

i0007

Temperature Dependent Dielectric Response of Ni Coated MWCNT/PVDF Nanocomposite

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Flexible and light weight nickel coated multiwalled Carbon Nanotube (Ni-MWCNT)/Polyvinylidene Fluoride (PVDF) Nanocomposite film is prepared by solution casting method to study its electrical transport mechanism. The inclusion of Ni-coated MWCNT nanofillers in the polymer leads to an improvement in dielectric features of the film. Temperature dependent AC conductivity follows Jhonscher's universal dielectric response. The analysis of the dielectric property of the parallel plate capacitive configuration of the nanocomposite is elucidated using modified Cole-Cole model.

i0009

Hot Electron Cooling in Disordered Graphene in BG Regime through Coupling with Flexural Phonons

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We have studied the hot electron cooling rate F(T) in disordered graphene in the Bloch-Gruneisen regime due to coupling with flexural phonons using Keyldysh Green's function method. The cooling rate is calculated as a function of temperature (*T*) and mean free path (*l*). We obtain analytical results for F(T) in both the impurity and clean limits. Also, from the complete numerical evaluation of the integrals, we find that the temperature dependence of the F(T) is sensitive to the presence of disorder as disorder suppresses temperature dependence of F(T), changing the power law from T^2 to $T^{5/2}$. Also, at very low temperatures, F(T) with flexural phonon couplingis found to be smaller than F(T) due to acoustic phonon coupling with electrons in disordered graphene. These calculations not only indicate the influencing effect of flexural phonon coupling on the transport properties of Dirac Fermions at very low temperatures with impurities but also provide a comparative behaviour with that of acoustical phonons due to deformation potential coupling.

i0010

High Temperature DC Electrical Transport Property of Polyvinylidene Fluoride Flexible Film

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Pure Polyvinylidene fluoride (PVDF) has been prepared by solution casting method. The film is characterized by FTIR and PL technique and the surface morphology is studied by AFM analysis. The temperature variation of the DC conductivity of the film reflects the semiconducting behavior with theoretical VFT model fitting. The resistance-voltage

characteristic of the flexible film shows hysteresis loop, leads to charge storage as well as memory device application of the film.

i0011

Extremely High Magnetoresistance in Perfect Electron-Hole Compensated WTe_2 Weyl Semimetal

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We have grown high quality single crystals of WTe2 and studied its bulk properties. The Magnetoresistance of this sample is found to be as high as 5.1×10^5 % at a temperature of 2 K and applied field of 12 T. Kohler's plot indicates the presence of two types of charge carriers and a perfect e-h compensation is proposed based on H^2 fitting. Shubnikov-de-Haas (SdH) oscillations have been observed for temperature up to 10 K. Single peak feature in the Fast Fourier transform (FFT) of these data establishes perfect e-h compensation in the sample.

i0012

Electronic and thermoelectric properties of *p* type $CeFe_4Sb_{12}$

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The study of electronic and thermoelectric properties of $CeFe_4Sb_{12}$ was studied considering generalized gradient approximation (GGA) as exchange correlation functional using density functional theory. The sample material revealed the degenerate *p*-type semiconducting nature with an energy gap of 0.21 eV. The positive magnitude of Seebeck coefficient predicted holes to be the majority of charge carriers. The computed value of Seebeck coefficient at room temperature was found to be 79.1 μV/K, which is close to that experimental result. The nature of electrical conductivity suggested the degenerate behaviour of the sample alloy. The sample compound revealed lowest lattice thermal conductivity of 0.68 W/m-K with maximum *ZT* value of 0.53 at 800 K.

i0014

Effect of Mo Doping on the Electrical and Magnetic Properties of Antiferromagnetic CrSe

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We report on the synthesis of Mo doped$Cr_{1-x}Mo_xSe$ (x=0.0, 0.01, and 0.03) polycrystalline samples using the solid-state reaction method. Room temperature powder X-ray diffraction (XRD) results suggest that all the samples are formed into the hexagonal crystal structure with a space group of $P6_3/mmc$. Electrical resistivity measurements suggest that all the samples are metallic in nature. Magnetization measurements suggest for a mixed magnetic phase at low temperatures, means, weak ferromagnetism is found in addition to the antiferromagnetic ordering for the parent system. Mo doping leads to a couple of additional antiferromagnetic magnetic transitions. We further observed decreasing magnetic moment with Mo doping.

i0017

Structural and Optical Characterizations of Multiferroic $Y_{0.95}Ba_{0.05}Mn_{1-x}Ti_xO_3$ Manganites

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In this work, polycrystalline samples of $Y_{0.95}Ba_{0.05}Mn_{1-x}Ti_xO_3$ (with x = 0.0 and 0.05) were synthesized by solid-state reaction method and their structural and optical properties have been investigated. The powder XRD patterns of the prepared samples confirm the formation of the hexagonal phase of the samples having *P6₃cm* space group symmetry. The diffused reflectance spectroscopy analysis has been employed to evaluate the optical bandgap of the prepared samples. The bandgap is found to decrease for higher Ti^{4+} concentration (x = 0.05) sample.

i0019

Investigation of structural and dielectric properties of fluorosubstituted zinc phthalocyanine films for electronic application

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In the present work, organic semiconductor films of hexadeca-fluorinated zinc phthalocyanine ($F_{16}ZnPc$) have been deposited using thermal evaporation technique on indium tin oxide (ITO) substrate and subsequently characterized for structural and morphological studies using Raman and field emission scanning electron microscopy (FE-SEM) techniques. Furthermore, dielectric and a.c. electrical characteristics have been analysed in the frequency range from 1 KHz to 1000 KHz at room temperature. The results on ac-conductivity reveal that conduction mechanism in film is found to be hopping transport model of charge carriers.

i0020

Optical and electrical transport properties of flexible PVA-chitosan-hematite composite film

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Hematite (α-Fe_2O_3) nanoparticles have been synthesis by hydrothermal method and photoluminance (PL) study shows a strong UV region's peaks make this hematite nanoparticle asa promising candidate for UV detector. The crystallite size of the hematite nanoparticles is 48 nm and the polymer composite with hematite nanoparticles reflects the semicrystalline behavior of the film. The ac conduction study reveals the charge carriers within the composite film follow the CBH model and the maximum barrier height is 0.12 eV. This film can be useful as a charge storage device as the room temperature dielectric constant and dielectric loss at 1 kHz frequency are 104 and 0.59 respectively. The temperature-dependent J-E characteristic shows a prominent hysteresis loop, and it increases up to four orders with the rise of temperature from 303K to 383K.

i0021

Observation of charge density wave transition in V-doped Bi2Se3

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Here we report the charge density transition in the Vanadium (V) -doped Bi2Se3 single crystals. The V-doped Bi2Se3 crystals were grown using a chemical vapor transport (CVT) method. Structural and compositional properties were confirmed by performing X-ray diffraction (XRD) and X-ray photo-electron spectroscopy (XPS). The four-probe resistivity measurement has been carried out in a low temperature cryostat down 5 K temperature. The variation of resistivity with temperature shows the pure metallic behavior with an anomaly around 250 K, the characteristic signature of charge density wave (CDW) transition.

i0022

An A*b-Initio* Study Of Electrical And Thermal Transport Properties Of FeXBi (X = Nb and Ta) For Thermoelectric Applications

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We investigated thermoelectric properties of 18-VEC half-Heusler (hH) alloys FeNbBi and FeTaBi under the framework of Density Functional Theory (DFT). Both hH alloys have a positive Seebeck coefficient, indicative of the p-type behaviour. The electronic feature suggests that the p-type doping at Bi-site will be more beneficial for achieving low lattice thermal conductivity. At 700 K, FeTaBi shows almost similar values on either p-type or n-type doping. Interestingly, at 1100 K, both the systems are found to have good power factor values. Overall, our results suggest potential new candidates of bismuth-based ternary compounds for high thermoelectric performance.

i0023

Structural, Electrical And Mössbauer Study In $Co_{1-x}Fe_xS_2$ ($0 \leq x \leq 1$)

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The results of X-ray diffraction, Mössbauer spectroscopy and resistivity measurements of $Co_{1-x}Fe_xS_2$ ($0 \leq x \leq 1$) are presented. The unit cell parameter follows Vegard's law across the series. The change in sign of temperature coefficient of resistivity around magnetic transition has been observed for intermediate compositions. Our Mössbauer studies show that both isomer shift and quadrupole splitting are correlated with electrical and structural measurements. Both the parameters vary linearly without any sign of discontinuity over entire composition range.

i0024

Optical, Electrical and Transport Properties of α-In_2Se_3 Crystal

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In_2Se_3 is an emerging 2D layered semiconductor which exists in different phases such as hexagonal and rhombohedral. We have synthesized single crystalline α-In_2Se_3 adopting a solid-state route with an optimized temperature profile. The phase purity of α-In_2Se_3 were

investigated by XRD and Raman measurements. To understand crystal anharmonicity and thermoelectric application of α-In_2Se_3, we have examined electrical and thermal transport properties. The estimated Seebeck coefficient, power factor, thermal conductivity, and Grüneisen parameter are ~ -173.74 μVK^{-1}, ~ 2.47 × 10^{-5} $Wm^{-1}K^{-2}$, ~ 1.35 $Wm^{-1}K^{-1}$ and ~ 1.29 respectively at 300 K. Combined high Seebeck coefficient and reduced thermal conductivity suggest α-In_2Se_3 to be potential thermoelectric material.

i0025

Magnetodielectric Coupling And High Frequency Relaxation Behaviour Of Neodymium Doped Nickel Ferrite Nanoparticles

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The Rare earth material, neodymium doped nickel ferrite nanoparticles are synthesized by sol-gel technique. The effect of doping of rare earth material in electrical transport properties is studied. The dielectric permittivity enhances with the doping of Nd atoms. Complex electric modulus spectroscopic analysis shows the non-Debye type relaxation behavior of the material, and the relaxation peaks are widened with temperature. The Room temperature magneto-dielectric coupling nature of the material exhibits a particular applied magnetic field value where the dielectric response is maximum. The doping of neodymium ions in nickel ferrite improves the magneto-dielectric response of the sample due to the crystalline strain induced.

i0026

High pressure structural and resistance study on quasi 1D compound Sr_2CuO_3

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This report presents the pressure dependence of structural and electrical transport properties of Sr_2CuO_3 investigated via synchrotron-based powder x-ray diffraction (XRD) and resistance measurement using diamond anvil cell (DAC) at low temperature. Sr_2CuO_3 shows structural stability up to the highest pressure of our study (~18GPa), but highly anisotropy in axial compressibility, c-axis being the soft axis. The temperature dependence of resistance shows an insulating nature up to the highest pressure of our study with systematic decrease in activation energy. The application of further high pressure may turn this compound in to a metallic state.

i0027

I-V Characteristics of Si PIN Diodes under Controlled Humid Conditions and Surface Passivation Layer's Integrity

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This work presents an investigation on reverse current-voltage (I-V) characteristics of commercial planar Si p-i-n (PIN) diodes from 0 to 100 V in ambient and controlled humidity conditions (Relative Humidity (RH) range from ~ 16 % to ~ 92 %). The reverse I-V characteristics of the diodes showed differences in reproducibility for different diodes of the same batch. Similarly, experiments performed for both the adsorption and desorption cycles

showed differences in the reversibility of the I-V characteristics for different diodes. These behaviors are attributed to the differences in the integrity of the surface passivation layer in terms of the pores and are further corroborated using Depth-resolved Doppler broadening studies using positron beam.

i0028

Studyof structural and transport properties of Al substitutedFe$_2$TiSn

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The structural, transport and magnetic properties of an otherwise nonmagnetic full Heusler alloy, Fe$_2$TiSn, is studied using Al doping at Sn site. The pristine Fe$_2$TiSn is prone to Fe-Ti antisite disorder that gets reflected in the upturn in ρ(T) data for T < 25 K. With Al doping, the upturn in the resistivity decreases, which could be because of magnetic order present in the samples.

i0029

Estimation of Band Offsets and Quantum Transport Properties Study of GeSn Nanowire

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One dimensional semiconducting core-shell nanowires (NWs) have attracted a large attention due to its potential application in high mobility FETs, semiconductor-superconductor hybrid devices and spintronics devices. In the present work, we have reported electronic and quantum transport properties GeSn core-shell NW. The GeSn-NW shows direct band gap semiconducting behaviour. Further, we have estimated the band offset of NW and studied their transport properties. We have observed linear characteristics behavior in I-V graph for the GeSn nanowire. Our study could motivate experimental researchers to fabricate this new composition core/shell nanowire.

i0030

Topological Hall effect in a centrosymmetric Gd$_2$PdSi$_3$ single crystal

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Topologically non-trivial magnetic structure, skyrmion, can be observed in crystal with broken inversion symmetry due to presence of Dzyaloshinskii-Morya interaction. Here we report the existence of strong topological contribution in the Hall effect measurement in a centrosymmetric crystal Gd$_2$PdSi$_3$ grown using Czochralski pulling technique. Gd$_2$PdSi$_3$ crystallizes in *AlB$_2$*-type structure. The topological contribution persists only within a short window of temperature and magnetic field, that was initially identified as the skyrmion phase, stabilized by mainly geometrical magnetic frustration. Specific heat measurement shows evidence of magnetic transition corresponding to antiferromagnetic ordering and huge change in magnetic entropy.

i0031

Effect of Mn concentration on the anomalous Hall effect in Mn_3Sn single crystals

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In ferromagnetic conductors, a transverse voltage drop appears even in zero magnetic field. This anomalous Hall effect is generally observed to be proportional to the magnetization, and thus is not typically observed in antiferromagnets in zero field. Mn_3Sn, an antiferromagnet has been shown to exhibit a large anomalous Hall effect by Nakatsuji et al with anomalous Hall conductivity reaching the same order of magnitude as in ferromagnetic metals. Also, it has a weak and soft ferromagnetic moment which switches the sign of the Hall Effect with a small magnetic field of around a few hundred oersted. We attempted to grow the single crystal of Mn_3Sn to study its anisotropic behaviour. However, the phase diagram of Mn and Sn shows that the crystal formation is still possible when the stoichiometry is not exactly 3:1. The details of crystal growth and its anisotropic physical properties and the effects of Mn concentration has been investigated in this study.

i0032

Crystal Growth and Mobility Fluctuations Driven Linear Magnetoresistance in YSi

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Linear magnetoresistance has been studied extensively over a wide range of phases from trivial to topological materials. In this report, we present the results on YSi single crystal growth and the anisotropic transport properties. YSi crystallizes in orthorhombic crystal structure with space group *Cmcm* (SG. No. 63). Resistivity measurements have been carried out along all three principle crystallographic directions, along $J \parallel [001]$ $\boldsymbol{B} \parallel [100]$ orientation linearity in magnetoresistance is observed for above ~10 T magnetic field. The linear magnetoresistance in YSi is caused by the mobility fluctuations that is explained by the famous Parish-Littlewood (PL) model.

i0033

Crossover from Linear to Quadratic Magnetoresistance in $NiTe_2$

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We have performed electrical transport and magneto-transport measurements on $NiTe_2$ single crystals and calculated the Debye temperature $\Theta_D \approx 230$ K using the extended Bloch-Grüneisen (BG) formula. The resistivity data fitting with BG indicates that resistance in this system is dominated by s-d electron-phonon scattering. Also, from the magnetoresistance (MR) measurements we observe a crossover from the linear magnetoresistance dependance on B ($MR \propto B$)to a quadratic magnetoresistance dependance on B ($MR \propto B^2$) at applied magnetic fields of B≈3.5 T and B≈-3.5 T.

i0034

Transport Properties of $Sb_2X_2Te_6$ (X=Si, Ge, Sn): A DFT Study

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Aim of this work is to probe the effect of isoelectronic substitution on $Sb_2X_2Te_6$ (X = Si, Ge, Sn) on the Seebeck Coefficient (S). We have optimized the structure of $Sb_2X_2Te_6$ (X = Si, Ge, Sn) by using the density functional theory based first principles calculations. Seebeck Coefficients of the probed systems have beencalculated using the semi-classical Boltzmann Transport equation. Further, we have compared the S values of $Sb_2X_2Te_6$ (X = Si, Ge, Sn) for p-type doping.

i0038
Strain-induced Anomaly And Chirality-dependent Planar Hall Effect In Type-II Weyl Semimetals
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Application of strain in Weyl semimetals (WSMs), quite remarkably, generates pseudo-electromagnetic fields and various novel anomalies. The planar Hall effect (PHE), occurring in regular WSMs, is one of the fundamental manifestations of of chiral anomaly. A major quest, therefore, is whether PHE could still arise in a strained type-II WSM without chiral anomaly. Using Boltzmann transport theory, we show that PHE does indeed appear in type-II WSMs solely from strain. The pseudo-magnetic fields couple to the Weylnodes of opposite chirality with opposite sign, leading remarkably to a finite chirality-dependent planar Halleffect (CPHE). We predict that a pure CPHE is possible even when PHE is absent for a particular strain configuration. We also discuss possible experimental detections of CPHE using circular dichroism.

i0039
Double Dielectric Relaxations in $Pr_{0.5}Ca_{0.5}Mn_{0.9}V_{0.1}O_3$ Perovskite
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We present the dielectric permittivity and electric modulus analysis of $Pr_{0.5}Ca_{0.5}Mn_{0.9}V_{0.1}O_3$ (PCMVO) perovskite compound, synthesized by solid state reaction method. Dielectric permittivity (ε') (also $d\varepsilon'/dT$) portrays the charge ordering and magnetic transitions behavior. Two relaxations are found around 45 K and 85 K. Arrhenius fitting revealed that, the low temperature relaxation is associated with the polaron hopping and the high temperature one is related to Maxwell-Wagner relaxation.

i0040
Magneto-transport properties of compensated metal PrSb
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We present the magneto-transport properties of PrSb single crystals. Magnetic-field-induced turn-on behavior and low temperature resistivity plateau have been observed.At 2 K and 9 T, a large, non-saturating transverse magnetoresistance (MR) 3.5×10^5 % has been obtained.

MRs followed Kohler's scaling.From the semiclassical two-band fitting of Hall resistivity, high carrier mobilities and almost equal electron and hole densities are deduced, which may result in large MR.

i0041

Role of Anions in Microscopic Dynamics in Acetamide Based Deep Eutectic Solvents

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Deep eutectic solvents (DESs) have been extensively studied over the last couple of decades owing to growing interest in their industrial applications The structure-dynamics relationship in these systems have shown interesting insights on the emergence of transport properties. Unraveling the correlation between hydrogen bond structure and microscopic dynamics of these systems can be a useful to tailor their bulk properties. In this study, we use quasielastic neutron scattering to explore the modulation diffusive dynamics of acetamide in various DESs. The results of the study show that the identity of anions in the DES, significantly alters the diffusion of acetamide, establishing the varying strengths of hydrogen bonding in the presence of different anions.

j: SEMICONDUCTOR PHYSICS

j0003

Growth of ultra-smooth molecular semiconductor and its structural analysis

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High performance of organic thin film transistors (TFT) requires uniform and ultra-smooth surfaces and interfaces. Here, we deposited Dinapthothienothiophene (DNTT) molecular film by effusion cell at high vacuum on a SAM functionalized dielectric. The SAM layer reinforce oriented growth of molecules and create ultra-smooth films of roughness 0.4 nm. X-ray diffraction revealed that molecules are oriented perpendicular to the substrate surface in (001) direction, which is required for the speedy motion of the charge carriers**.**

j0004

Optimization of Post-Treatment Annealing Conditions for RF Sputtered CIGS Thin Films

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A new approach was adopted for the post-processing of CuInGaSe2 (CIGS) thin films deposited using single target sputtering method. The as-sputtered samples were annealed in muffle furnace and rapid thermal processing (RTP) chamber with successive higher and lower temperature cycles at 450 °C for 10 minutes. The samples were analyzed for structural and optical properties. RTP treated samples revealed better results compared to the annealed sample. Rietveld refinement gives the c/a value 2.005 (close to the ideal tetragonal crystal) in RTP treated sample. Optical measurement shows the increased absorbance values in RTP treated sample than furnace annealed sample. The bandgap was estimated to be 1.34, 1.22 and 1.18 eV for as-sputtered, annealing and RTP treated sample. Our experiment shows, however, the similar parameter used for annealing, RTP treated sample shows better results.

j0005

Influence Of Different Ion Fluence On The Structural And Optical Properties Of $Bi_5In_{30}Se_{65}$ Thin Films

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The present paper reports the effect of different fluence of proton ion irradiation on the optical and structural properties of $Bi_5In_{30}Se_{65}$ thin film. The studied thin films were prepared by the thermal evaporation technique from bulk material and irradiated with 30KeV proton ions with three different fluences. The XRD study revealed that ion irradiation led to retain its amorphous nature with increasing fluence. However, the UV-visible spectroscopy revealed the reduction in the optical band gap and transmittance with increase in ion doses. This decrease in the optical bandgap is due to the increase in the lattice defects with ion irradiation. The corresponding changes in the surface structure have been observed from the AFM study.

j0008

Depth Profile Analysis of Gold Ions in Silicon <100> Substrate

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Ion implantation is a popular method for introducing foreign species into a target material. It transforms the structural, optical, electrical, and magnetic properties of the target materials, resulting in the creation of a new material. The implantation of gold ions in silicon results in improved sub-band gap characteristics, which has a wide range of applications in the field of optoelectronic device and infrared detectors. Miniaturization of semiconductor devices often necessitates an exact and precise depth distribution of implanted ions within the crystalline silicon substrate. In the present work, we have used a non-destructive approach to analyse the depth distribution of gold ions implanted in silicon <100> substrates using combined X-ray reflectivity and grazing incidence x-ray fluorescence measurements.

j0010
Structural and dielectric properties of $SrSnO_3$ and $SrSn_{0.98}Ti_{0.02}O_3$
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The sample $SrSnO_3$ and $SrSn_{0.98}Ti_{0.02}O_3$ are synthesized using chemical route followed by heat treatment at 1173 K. Rietveld refinement analysis performed on XRD data of samples has been indicated that the samples are crystallized into orthorhombic phase under space group Pbnm. The lattice constants and X-ray density are decreased with Ti^{4+}. The dielectric properties indicate the existence of interfacial and orientation polarization in samples. The dielectric constant and tangent loss are found to be thermally stable up to 300°C that makes it potentially application for thermally stable capacitor and electrical device applications.

j0011
Bi-functional behaviour of ZnO/RGO/Au device: Photodetector as well as light induced memory device
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We have investigated photo-response as well as resistive switching behaviour in hybrid zinc oxide (ZnO)/reduced graphene oxide (rGO) bilayer thin film, prepared through sol-gel process on an ITO coated glass substrate under dark and illumination condition of light. It has been observed that impedance value decreases with the increase in light intensity. Real and imaginary part of impedance are observed to maintain saturation up to a knee frequency which decreases with further increase of frequency up to the highest experimental limit. These results indicate the higher generations of photo generated carriers at the interface between rGO and ZnO layer and an enhancement of the charge transport process due to the increment of the mobility of charge carriers in the system.

j0012
Electric field-induced hysteresis observed in thiol-ene-epoxy based polymeric devices
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In this work, an off-stoichiometry thiol-ene-epoxy polymer based metal-semiconductor-metal device was fabricated on planar interdigitated electrodes. The presence of ferroelectric dipoles was observed at room temperature when electric field-assisted current-voltage (I−V) was measured. The hysteresis loop in I-V was measured to understand the effect of dipoles. The presence of ferroelectric dipoles in OSTE+ polymer is beneficial for memory application

j0014
Influence of Buffer Layer on Physical Properties of RF Sputtered ZnO:Mo Films on Flexible Substrate
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Mo doped ZnO thin films (MZO) have been prepared by RF sputtering technique on PET substrate to study the influence of substrate temperature and buffer layer on the physical properties. With an increase in the substrate temperature, the crystallinity of the films has been improved. All the films show average 85% transparency in the visible region. The buffer layer helps to grow the film along <002> orientation resulting in better electrical property with the lowest and stable sheet resistance of 760 Ω/sq.

j0016
Grain Size Dependent Thermoluminescence Characteristics Of Beta-Irradiated Diamond Films
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We report on the effect of grain size on the thermoluminescence (TL) characteristics of diamond films. The diamond films with different grain sizes in the range of 0.02 - 1.5 μm are grown by hot filament chemical vapour deposition. The graphitic carbon content in the diamond films increases with reduction in grain size as evidenced by Raman spectroscopy. Upon beta-irradiation, the TL glow curves of these diamond films display two prominent peaks ~ 100 and 290 ^{O}C corresponding to two different trap and recombination centers. The TL characteristics are discussed in terms of structural defects in diamonds.

j0018
Development of CsI(Tl) Coupled GaAs Detector for γ-ray Detection
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In this work, the performance of an indigenously developed γ-ray detector is presented. The detector consists of a CsI (Tl) single crystal scintillator optically coupled to GaAs photodiode. The single crystal of CsI (Tl) and GaAs photodiode structures are grown by Bridgman technique and MOVPE respectively. The measured optical response of the individual components confirms their suitability for device integration. At 300K, measured dark current of the developed detector is 1.14 nA. Exposure to a γ-photon flux of 10^7ph/s/mm^2 on CsI (Tl) led to the generation of 10^{11}ph/s/mm^2 visible photons of 2.27 eV which produced nearly 32.44 nA electrical signal at an applied reverse bias of 3V.

j0019

Temperature Dependence Of Band Gap Of β-$(Al_xGa_{1-x})_2O_3$ Alloys From Optical Reflectivity

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Band gap variation of β-$(Al_xGa_{1-x})_2O_3$ alloys with temperature has been studied to investigate the electron-phonon interactions. The obtained value of mean phonon temperature lies in between 473 K - 488 K, which corresponds to the involvement of phonons mainly related to deformation of [GaO_4]/ [AlO_4] tetrahedrons and [GaO_6]/ [GaO_6] octahedrons (300-500 cm^{-1}) group.

j0020

Transfer Matrix Method for Reflectivity Simulation of Distributed Bragg Reflector (DBR)

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Distributed Bragg Reflector (DBR) is multilayered structure comprising materials having different refractive indices. Reflectivity of such DBR depends on the difference between the refractive indices (RI). Therefore, selection of suitable materials is challenge in construction of DBR. In this paper reflectivity of DBRs constructed using various II-VI various compound semiconductors is simulated using Transfer Matrix Method (TMM). The simulation is carried out for various combinations such as ZnTe/ZnSe, ZnTe/CdSe, ZnTe/CdTe, ZnSe/CdSe, CdTe/ZnSe by MATLAB software. The reflectivity is simulated for 20 periods and at an incident angle of 0^o and 45^o

j0021

Study of Thermal Decomposition of Sb_2Se_3 Crystal

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Sb_2Se_3 crystal has been grown by direct vapour transport (DVT) technique. The elemental composition of the grown crystal was analysed by energy dispersive X-ray analysis (EDAX). The kinetic decomposition parameters of the crystals have been studied by thermogravimetric analysis (TGA). The TGA thermogram shows single stage decomposition. The activation energy of kinetic degradation has been determined by Broido, Coats-Redfern and Horowitz-Metzger approximation methods. The analysis shows that the grown crystals have excellent thermal stability and it is also applicable in thermoelectric generator.

j0022

Role of precursor parameter on structural and optical studies of sol-gel grown GaN

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GaN has been grown by varying precursor concentrations using the sol-gel technique. The influence of varying concentrations on structural, morphological, and optical characteristics was studied. X-ray diffraction and Transmission Electron Microscopy shows the wurtzite structure and highly crystalline nature of the GaN nanostructure. SEM image shows the hexagonal structure for lower concentrations and nanorod for 1M concentration. The photoluminescence study shows the optical band gap of 3.3 eV to the grown GaN nanostructure.

j0023

Micro Raman Studies on HVPE Grown GaN epi-layers Irradiated with Light Ions

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The hydride vapor-phase epitaxy (HVPE) grown GaN epi-layer was irradiated with 100 MeV O^{7+} for different fluences. In this paper, the structural aspects of pure and irradiated sample has been investigated using micro Raman Spectroscopy by the Lorentz peak fitting method. The allowed Raman modes E_2^H and A_1 (LO) for wurtzite structure is observed for all the samples. The Carrier Concentration (n), biaxial stress (□) are calculated for the pure and irradiated samples and the results are compared. On increasing the fluences the carrier concentration increased and the biaxial stress decreased. The wurtzite structure of GaN has been ascertained from the X-ray diffraction (XRD) analysis though it was found that the intensity of the peak reduced for their irradiated sample.

j0024

Site Selective Non-Stoichiometry Study Of $LaAlO_3$

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Sol-gel synthesis method has been used to synthesize $LaAlO_3$ with non-stoichiometry at Lanthanum (La/A-site) and Aluminum (Al/B-site) sites. The pure phase of samples has been optimized at 900ºC and confirmed by X-ray diffraction technique and Rietveld refinement

analysis. Decrement in the lattice parameters has been observed in non-stoichiometric samples compared to pure $LaAlO_3$ systems. Interestingly, decrease in band-gap values has been observed with the non-stoichiometric approach. This study demonstrates that slight disturbance at La and Al sites can enhance the physical properties of the pristine $LaAlO_3$ system.

j0026

Robust P-type Conduction in Oxychalcogenides CuAlOS: A DFT Study

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The study reveals the structural, electronic and optical properties of oxychalcogenide compound CuAlOS using first principles calculations based on density functional theory (DFT) implemented in quantum espresso code. This compound possesses the same crystal geometry ($R\bar{3}m$) like most of the delafossite compounds. The calculated electronic band structure reveals the semiconducting nature of the considered compound having electronic band gap of 0.27 eV. Furthermore, we have calculated partial density of states (PDOS) to see the contribution of 3d and 2p orbitals, which are mainly responsible for the lower electronic band gap. Additionally, the optical properties such as dielectric constants, absorption spectra and refractive index were calculated to confirm the applicability of the nominee compound in the optoelectronics.

j0027

A Facile Approach to Improve ON/OFF Ratio and Uniformity of Low-power HfOx based RRAMs

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The resistive switching performance of hafnium oxide-based devices with transparent conducting oxides as bottom electrodes is investigated. The sputtered HfO_x film exhibits a typical clockwise-bipolar resistive switching with lower forming voltage, SET/RESET voltages, appreciable ON/OFF ratio, and self-compliance effect. Further, a simple method inspired by the hot-forming technique to suppress the current overshoot and better control the conductive filament formation and dissolution inside HfO_x films of Al/HfO_x/FTO and Al/HfO_x/ITO devices is proposed. By implementing this method, the ON/OFF ratios of Al/HfO_x/FTO and Al/HfO_x/ITO devices are improved. Moreover, the ON/OFF ratio and temporal variability could be further tuned by the modulation of the thickness of HfO_x layer

j0029

Light Stimulated Artificial Synapses Based on Polymer Semiconductors PBTTT and PFO

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The development of synaptic devices with polymer semiconductor has drawn great attention to meet the requirement for fabricating human brain like computing and soft robotic system for artificial intelligence-related research. Taking advantage of the properties of organic semiconductors like low cost, easy solution possible, large area fabrication and biocompatible are attractive features for artificial synapses. In this study, two terminal synaptic devices are fabricated using the PBTTT and the PBTTT: PFO system. Biological synapse like nature, short-term plasticity (STP), pulse pair facilitation (PPF) and memory-forgetting-rememorizing (MFR) behaviour are successfully carried out. We attribute the behaviour of this device of charge trapping mechanism in PBTTT:PFO material system.

j0030

Low-temperature Solution-processed ZrO_2 and Ta_2O_5 for High-performance Solution-processed Organic Field-effect Transistors

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Low-voltage operation of solution-processed organic field-effect transistors (OFETs) is very important for the integration of these devices into complex integrated systems. Owing to low dielectric constant and high density of trap centers, the use of conventional dielectric SiO_2 generally leads to large operating voltage in organic field-effect transistors. Here, we have demonstrated low-temperature solution-processing of zirconium oxide (ZrO_2) and tantalum oxide (Ta_2O_5) for their use as gate-dielectric in solution-processed organic field-effect transistors. ZrO_2 and Ta_2O_5 have significantly larger dielectric constant than SiO_2. The field-effect mobility in PBTTT-C14 improves from 2.73×10^{-3} cm^2 V^{-1} s^{-1} for SiO_2-gated OFETs to 1.65×10^{-1} cm^2 V^{-1} s^{-1} and 3.02×10^{-1} cm^2 V^{-1} s^{-1} for ZrO_2 and Ta_2O_5 gated OFETs respectively. The threshold voltage decreases significantly from ~ 24 V for SiO_2-gated OFETs to ~ 0.15 V and ~ 0.03 V for ZrO_2 and Ta_2O_5 gated OFETs respectively. The low-temperature processing enables this technique to be used for flexible substrates also.

j0032

Study of Interface phonons in InAs/$GaAs_{1-x}Sb_x$ Quantum Dot Heterostructures by Low-temperature Polarized Raman scattering

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An experimental study of interface phonons in bilayer strain-coupled InAs/$GaAs_{1-x}Sb_x$ quantum dot (QD) heterostructure has been presented by means of low temperature Raman scattering. The QDs were prepared with Sb concentration of ~ 10% (sample A) and ~20% (sample B) which results in transformation of band alignment from Type I to Type II at ~14 -16 %. The strain profiles in A and B were also theoretically simulated and the strains in sample B are found to be less than those for sample A and also the size of the QDs in B is wider. The Raman peak positions show shift from the ideal LO and TO values due to the presence of interface strain. The strains estimated from such shift in the Raman peak positions of different interface modes of InAs and GaAs QDs are in good agreement with the simulated values. The higher Sb content results in lower strain in B due to the lower lattice mismatch between the InAs and the $GaAs_{1-x}Sb_x$ capping layer. The interface Raman peaks show a

higher frequency shift in the heterostructure with higher Sb content which is attributed to the strain relaxation, bigger size of the QDs and type II band alignment.

k: MAGNETISM, SUPERCONDUCTIVITY, AND SPINTRONICS

k0001

Optical Coherent Transient Effects in Core-Shell Quantum Dots

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We present the results of the numerical analysis of the third order optical non-linearity and optical coherent transient effects like optical nutation in various Type-I core-shell quantum dots at low temperature and in ultrafast, moderate power coherent excitation regime. We have considered the role of Wannier-Mott excitons since they are more pronounced in semiconductor nanostructures. The dephasing and relaxation mechanism of excitons is also incorporated in the theoretical model.

k0002

Improving the Magnetic properties of Neodymium Doped $CoFe_2O_4$ Film by Nebulizer Spray Method

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Doping of rare earth element with $CoFe_2O_4$ thin films can make significant changes on the structural and magnetic properties, which makes it suitable for magnetic and other device applications. Undoped and neodymium doped $CoFe_2O_4$ thin films were deposited using Nebulizer Spray Pyrolysis (NSP) on glass substrates by varying Nd doping level from 0% to 5%. From X-ray diffraction pattern, crystallite size is calculated and is found that the crystallite size decreases with the doping concentration. The calculated optical band gap values exhibits an increasing trend and shifted from 1.82 to 1.95 eV on increasing Nd doping concentration. The magnetic and the saturation magnetization of the films obtained at 0% and 5% showed a strong dependence on the Nd doping concentration

k0003

High Temperature Structural Properties of $Bi_{1-x-y}La_xSr_yMnO_3$ (x = 0.0, 0.1; y = 0.3, 0.4)

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High temperature X-ray diffraction studies have been carried out on a series of substituted $BiMnO_3$ samples. With the changes in the composition of Bi and Sr, it is found that though there is no change in crystallographic structure, there are subtle changes in the unit cell parameters and lattice distortions which could be responsible for the differences or modifications in the physical properties of these compounds.

k0004

Influence of Slow Cooling and Magnetic Properties of Fe-Ga Alloy

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The structural and magnetic properties of Fe_{77}-Ga_{23} alloys were investigated after they were arc melted and heat treated at 900 °C. for 5 hrs followed by furnace cooling. The results of X-Ray Diffraction study confirm the alloy's Body Centered Cubic structure and the presence of the A2 phase. Optical microscopy study also confirm the presence of equiaxed grains of only single phase (A2). Additionally, differential scanning calorimetry confirms the existence of the A2 and DO_3 phases. Vibrating sample magnetometer was used to determine the saturation and remanent magnetization.

k0005
Hierarchical Relaxation In The Vortex Matter Of Superconducting $Nb_{99}Zr_{01}$ Alloy
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We report experimental studies on relaxation dynamics in the superconducting state of $Nb_{99}Zr_{01}$ as-cast alloy. Magnetization was measured as a function of time at a fixed temperature of 2K under various magnetic field values. The non-exponential relaxation of magnetization is described within a framework of interacting clusters that leads to hierarchical relaxation. Our work reported here suggests that clusters of flux lines (flux bundles) which interact with each other, participate in the relaxation process instead of single isolated flux lines. The observation of hierarchical relaxation indicates a continuously evolving landscape of the underlying pinning potential.

k0006
Synthesis and Characterization of Sugar Coated Superparamagnetic $Zn_{0.5}Fe_{2.5}O_4$ Nanoparticles
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Sugar coated superparamagnetic $Zn_{0.5}Fe_{2.5}O_4$ nanoparticles are synthesized by sugarcane juice mediated green sol gel route. Phase pure partially inverse spinel ferrite type fcc spinel structure of sugar coated $Zn_{0.5}Fe_{2.5}O_4$ nanoparticles of ~22nm is confirmed by XRD, FTIR and Raman spectroscopic measurements. $Zn_{0.5}Fe_{2.5}O_4$ nanoparticles absorb considerable light in UV and visible region and exhibit semiconducting behaviour with a band gap of ~1.7 eV. Presence of Fe^{3+} ions in high spin state have been validated by ESR study. Field dependent magnetization data showed superparamagnetic character of $Zn_{0.5}Fe_{2.5}O_4$ nanoparticles with a saturation magnetization of 37emu/g at 300K. Sugar coating on $Zn_{0.5}Fe_{2.5}O_4$ nanoparticles is established by the difference in average crystallite size and the size of magnetic nanoparticles obtained using lognormal distribution. Sugar coated $Zn_{0.5}Fe_{2.5}O_4$ nanoparticles are semiconducting and superparamagnetic at 300K.

k0007
The *ΔH-M* and *ΔM-H* techniques to understand the magnetic biasing in magnetic composite
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Composite of $BaFe_{12}O_{19}$ (BHF) and $CoZn_{0.25}Fe_{11.75}O_4$ (CZFO) exhibits magnetic biasing, i.e., the influence of two magnetic phases on each other. This magnetic biasing in magnetic composites is the center of discussion for the last few decades to tune the magnetic parameters for technological applications. But there is no direct method to understand the magnetic interaction between two phases in the composite. This magnetic interaction is mostly due to surface interaction between two magnetic materials if they are below their spin coherence length. In the present study, the loop width (ΔH)-Magnetization (M) and switching field distribution (a derivative of demagnetization with respect to applied field, ΔM-H) techniques have been employed to understand the magnetic biasing between BHF and CZFO in the composite. The present study opens a new window to understand the magnetic interaction between different magnetic phases in the composite.

k0008

Doping Induced Band-Renormalization in 122-type Fe-based Superconductor

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In this paper, we study the effect of doping on electronic structure of 122-type Fe-based superconductor (FeScs) using angle-resolved photoemission spectroscopy (ARPES). We find significant orbital-dependent band-renormalization with doping along with an enhanced spin-orbit coupling (SOC) strength leading to an increased band separation. Experimental results could be captured well using density functional theory. We find that pnictogen height plays an important role in the electronic structure.

k0009

Temperature dependence of reciprocal susceptibility in linear Mn chains of Ti_4MnBi_2

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We applied the self-consistent renormalization theory of spin fluctuations implemented with first principles calculations for a quasi-one-dimensional system: Ti_4MnBi_2. The inverse susceptibility is calculated at finite-temperature T and compared with the experimental data (*Phys. Rev. B* **102**, 014406, 2020). A Curie-Weiss fit to our results suggests that the Mn moments are in the low-spin half configuration and the estimated Curie-Weiss moment is pointedly reduced from Hund's rule value.

k0010

Characterization of unusual vortex-velocity fluctuations above unjamming threshold in 2*H*-NbS_2 superconductors

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Here, using 4-probe transport measurement, we investigate the unusual voltage (V) fluctuations above a non-equilibrium (NE) jamming/unjamming transition for a driven vortex matter in 2H-NbS_2. Analysing the time (t) series of voltage fluctuations ($V(t)$) at the unjamming threshold, we reveal signatures of negative vortex velocity events, where vortex flow seems to occur in a direction opposite to the drive. And we show that these unusual V-fluctuations obey Gallavotti-Cohen non-equilibrium fluctuation relations.

k0011

Ion Beam Mixing of Mn/Al Bilayer Thin Films: Structural and Magnetic Properties

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The ferromagnetic τ-phase was achieved in the Mn/Al bilayer thin films by Xe ion irradiation. Mn/Al bilayer thin films were deposited on Si substrate by evaporation technique for the total thickness of 95 nm. These as-deposited films were irradiated by 400 keV Xe ions with the fluences of 5×10^{16} and 1×10^{17} ions/cm^2. The enhanced ferromagnetic properties of the irradiated films are confirmed from the XRD, MFM, and VSM results.

k0013

Fe-Based Half Metallic Fe_2MnSi Heusler Alloy For Spin-Injection Devices

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Heusler alloys are ternary intermetallic alloys represented by the formula X_2YZ or XYZ, where X and Y is the transition metals and Z is the main group element. It possess half metallic behaviour, that is the majority spin band shows metallic behaviour and the minority spin band exhibits semiconducting behaviour with a band gap at the Fermi level, which is leads to 100% spin polarization. The Fe_2MnSi Heusler alloy was synthesized by solid state reaction method. X-Ray diffraction pattern represent the formation of $L2_1$ phase with cubic structure. The surface morphology of the sample was carried out using High resolution scanning electron microscope. The presence of Fe, Mn and Si in the alloy was confirmed by using Energy dispersive x-ray spectroscopy. From the elemental contrasting mapping it is proven that sample as fine distribution of Fe, Mn and Si. Magnetic property was studied using Vibrating Sample Magnetometer. The prepared alloy exhibiting soft ferromagnetic property with low coercivity (H_C) of 8.13 Oe. Hence it is suitable for spin-injection and spintronics device. Also, particularly Si containing full-Heusler alloys are promising materials for spin injector.

k0016

Magnetic Anomalies in Cubic R_4PtAl (R = Ho and Er)

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We report the results of magnetization, and magnetoresistance (MR) measurements down to 1.8 K on Gd_4RhIn-type cubic compounds, Ho_4PtAl and Er_4PtAl. There are three crystallographic sites for rare-earth (R) ion, providing an opportunity to understand magnetism in such a complex rare-earth environment. Dc magnetization data reveal that the magnetic ordering sets in around 21K and 12K in Er and Ho compounds, respectively. In addition, there is another magnetic feature around 17 K for Ho_4PtAl. Dc electrical resistivity exhibits a weak minimum at a temperature marginally above their respective T_N. There are fascinating findings in the isothermal magnetoresistance (MR) data, the most notable one being multiple sign-crossover for Ho_4PtAl, but not for Er_4PtAl, in the magnetically ordered state, suggesting possible subtle field-induced changes in the magnetic structure of the former. The results overall suggest that these compounds exhibit interesting magnetic and transport properties.

k0018
Low Temperature Structural Anomaly in $Pr_{0.6}Sr_{0.4}MnO_3$
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The compound $Pr_{0.6}Sr_{0.4}MnO_3$ undergoes magnetic ordering from paramagnetic state to ferromagnetic state just above room temperature, at T_C = 308K. In addition to room temperature magnetism, the compound exhibits another anomaly, that is drop in magnetic susceptibility at T = 89K. In order to understand the origin of this secondary feature, we carried out detailed low temperature x-ray diffraction measurements and find that the crystallographic structure changes from orthorhombic space group Pnma to mix of orthorhombic and monoclinic structure (space group I2/a). Our analysis shows that the transformation from Pnma to I2/a is incomplete down to 5K, resulting in phase coexistence of mixed structures below 150 K. Detailed analysis of the XRD patterns has been presented and discussed to understand the evolution of the structural transition.

k0019
Tailoring Magnetization Switching in Electrodeposited FeNi Films
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Magnetization switching modes in electrodeposited FeNi films have been tuned by providing suitable thermal agitation effects. Angular variation coercivity and magnetic microstructure analysis are used to examine the domain reversal mechanism as a result of annealing in an inert and reducing atmosphere.

k0020

Development of Mg Substituted Lithium Ferrite ($LiFe_5O_8$) for Microwave Applications

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Mg substituted lithium ferrites with improved dielectric response are synthesized by the conventional solid-state route. Reitveld refinement disclosed the generation of monophase spinel ferrites (space group – $P4_132$). Substituted ceramics exhibited uniform grain growth and maximum density. The dielectric constant is enhanced, and the dielectric loss is significantly reduced (10^{-3} order). A blend of low loss, high permittivity (ε_r = 3034), and excellent permeability (μ_r = 28) of LMFO made x = 0.005 specimens suitable for microwave applications.

k0021

Magnetic and Exchange Bias Properties of Bulk and Nanocrystalline $La_{0.375}Ca_{0.625}MnO_3$ Compound

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Magnetic properties and exchange bias effect of the polycrystalline and nanocrystalline $La_{0.375}Ca_{0.625}MnO_3$ compounds have been presented. With reduction of the particle size, uncompensated surface spin induced ferromagnetism is pronounced in nanocrystalline sample. However, at higher magnetic field value, long range charge ordering (associated with antiferromagnetic nature) is predominant even in nanoparticles similar as bulk counterpart. Exchange bias properties of both compounds have been found at low temperature with increasing nature depending on the cooling magnetic field. Modification in exchange bias properties in nanocrystalline sample is addressed considering the disordered polymorphs developed within the charge-orbital ordered phase.

k0022

Structural and Dielectric Characterization of $LiNbO_3$ Substituted $BiFeO_3$

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A polycrystalline lead-free sample having a composition of $Bi_{0.65}Li_{0.35}Fe_{0.65}Nb_{0.35}O_3$ (namely BLFO) is synthesized by a ceramic processing route. X-ray diffraction pattern taken at room temperature was employed to verify the formation of phase and unit cell parameters of the sample. The morphological analysis suggests a dense ceramic with non-uniform grain distribution. The dielectric properties of the material were analyzed at different interval of frequencies (10^2–10^6 Hz) and temperatures (20–480 ^oC) using impedance spectroscopy techniques. There is a presence of combined grain and grain boundary effects analyzed from this technique. The structural properties correlated with dielectric properties.

k0023

Magnetic Transition in $LaVO_3/LaTiO_3$ superlattice: A DFT+MC study

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Magnetic phase transitions have been explored in a superlattice formed by stacking monolayers of $LaTiO_3$ and $LaVO_3$ alternately, using ab-initio density functional theory (DFT) and Monte-Carlo (MC) simulations. DFT derived intra-layer and inter-layer exchange interaction parameters were used for the MC simulations on a Ising spin model Hamiltonian. Two sharp peaks observed in specific heat without the interlayer exchange coupling indicate two independent magnetic ordering in $LaTiO_3$ and $LaVO_3$ layers at different temperatures. Inclusion of interlayer coupling leads to one sharp peak at higher temperature with a broad hump like feature at lower temperature in specific heat indicating a single magnetic phase transition to *C-type* antiferromagnetic phase in the superlattice.

k0024

Structural and low temperature magnetic studies of M-type barium hexaferrite

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Barium hexaferrite ($BaFe_{12}O_{19}$) with hexagonal structure has been prepared by conventional solid-state method and calcined at 1000°C. XRD pattern confirmed the formation of single-phase, whereas EDX and elemental mapping reconfirmed the formation of barium hexaferrite. The obtained crystallite size (34.04 nm) is below < 50nm, making it suitable for magnetic recording. High coercivity is observed at both 300 and 5K. The giant coercivity (H_c = 2.19 kOe) and high saturation magnetization (M_s = 62.06 emu/g) are observed at 5K. Temperature variation ZFC and FC curve is also measured up to 300 K.

k0025

Effect Of Magnetic Field On Thermodynamic Properties Of Anderson Lattice Model: An Application To Colossal Magnetoresistive Manganites (Re_{1-X} Ax MnO_3)

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In the present investigation, by using variational method we have studied the effect of magnetic field on various thermodynamic properties like specific heat (C_v) & magnetic susceptibility (χ_s) etc. of rare earth manganites doped with alkaline earths namely Re_{1-x} A $_x$ MnO_3 (where Re = La, Pr, Nd etc., and A= Ca, Sr, Ba etc.) exhibiting colossal magnetoresistance (CMR) phenomena. We have used a two band (l-b) Anderson Lattice model Hamiltonian to study these materials in the strong electron-lattice Jahn- Teller (JT) coupling regime an approach similar to the two- fluid models. We find that both the quantities C_v & χ_s increase with increasing magnetic field 'h'& 'm' parameters showing the peak at intermediate values & finally decreases at higher values of h, m parameters. We have shown the curves at temperature 100 K & 300 K only. We have also observed the effect of doping concentration ' x ' on both C_v & χ_s. Both the quantities reduce as we increase the doping 'x'. The peak occurs near x=0.3 which shows the optimum value of x. Our results are in good agreement with the available experimental data.

k0026

Doping effects in Heusler superconductor, $ScAu_{2-x}M_xAl$ (*M*: Cu, Pt)

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Here, we report the effect of doping on lattice parameter (*a*) and superconducting transition temperature (T_c) in Heusler superconductor, $ScAu_{2-x}M_xAl$ (*M* : Cu (iso-valent doping) and Pt (hole doping)) with $x = 0.1$ and compare the T_c and *a* values with that of the parent compound. Rietveld refinement of the powder x-ray diffraction (XRD) shows decrease in lattice parameter (*a*) with doping. Further, from temperature (*T*) –dependent susceptibility measurement, we show decrease in T_c in doped compounds. We argue that the negative effects of doping on T_c are associated with change in phonon spectrum with doping.

k0028

Two-dimensional Short-range Magnetic Correlations in the Geometrically Frustrated Maple Leaf Lattice (*S*= 3/2) compound $Na_2Mn_3O_7$

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Two dimensional (2D) geometrically frustrated quantum magnets having new class of maple leaf lattice (MLL) are of current interest because of their novel magnetic behaviours. In the present study, microscopic understanding of the magnetic properties of $Na_2Mn_3O_7$ having MLL spin system have been investigated by using neutron diffraction study. The present compound exhibits pronounced quantum effects by showing absence of long-range magnetic ordering. In-depth understanding of spin-spin correlations are obtained by comprehensive Reverse Monte Carlo (RMC) analysis, which reveals that the magnetic spin-spin correlations are confined within the 2D MLL lattice planes in $Na_2Mn_3O_7$. The present study provides an insight on the magnetic correlations having new class of frustrated 2D maple leaf lattice geometry.

k0029

Growth temperature induced modifications in structure and magnetic anisotropy of magnetron sputtered FeCoB alloy thin films

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We report on the evolution of the structure and magnetic anisotropy of magnetron sputtered Si(100)/SiO_2/W/FeCoB thin films prepared at different substrate temperatures (Ts). Film deposited at Ts=300 K exhibits amorphous structure with well-defined uniaxial magnetic anisotropy (UMA) in the film plane. At Ts ≥ 673 K, FeCoB films have partially crystalline microstructure, where bcc-FeCo nanocrystalline grains are dispersed in remaining amorphous matrix. Increase in Ts leads to gradual disappearance of in-plane magnetic anisotropy. Coercive field (Hc) shows an increase from ~5 Oe to 63 Oe with growth temperature, though crystallite size remained in the range of 5-6 nm i.e., well below the

ferromagnetic exchange correlation length. The disappearance of UMA and increase in Hc with the growth temperature can be ascribed to change in the magnetisation reversal process with increasing surface roughness.

k0030

Ni Induced Ferromagnetism in Mn_3Ga

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Structure and magnetic properties of Mn_3Ga are dependent on annealing temperature. The high temperature (850°C) annealed Mn_3Ga is antiferromagnetic with a disordered fcc structure, while the tetragonal structure of the low temperature (400°C) annealed Mn_3Ga induces a ferrimagnetic ground state. Ferromagnetic interactions can also be induced by replacing Mn by Ni in the 850°C annealed alloys. A comparative study of the local structures of constituent atoms in these undoped and Ni doped Mn_3Ga alloys indicate structural distortions induced by Ni to be responsible for the ferromagnetism in the cubic alloy.

k0031

Influence of Annealing Temperature on Structural and Magnetic Properties of Nanoscale Fe, Mn: SnO_2 and Cr, Mn: SnO_2

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The influence of Fe and Mn co-dopants, Cr and Mn co-dopants and annealing temperature on the structural and magnetic properties of nanoscale SnO_2 were investigated via complementary experimental techniques. $Sn_{0.96}Fe_{0.02}Mn_{0.02}O_2$, $Sn_{0.92}Fe_{0.04}Mn_{0.04}O_2$, $Sn_{0.96}Cr_{0.02}Mn_{0.02}O_2$ and $Sn_{0.92}Cr_{0.04}Mn_{0.04}O_2$ were prepared by high pressure microwave synthesis technique and annealed at 500 °C for 2 h and 450 °C for 6 h. Powder X-ray diffraction (PXRD) pattern of both as-synthesized and annealed samples indicated the single-phase tetragonal rutile structure of SnO_2. Magnetic studies of as-synthesized samples revealed the paramagnetic nature at 300 K. The prepared $Sn_{0.96}Fe_{0.02}Mn_{0.02}O_2$, $Sn_{0.92}Fe_{0.04}Mn_{0.04}O_2$, $Sn_{0.96}Cr_{0.02}Mn_{0.02}O_2$ and $Sn_{0.92}Cr_{0.04}Mn_{0.04}O_2$ samples annealed at 500 °C for 2 h unveiled the room temperature ferromagnetism (RTFM). In addition, $Sn_{0.96}Cr_{0.02}Mn_{0.02}O_2$ and $Sn_{0.92}Cr_{0.04}Mn_{0.04}O_2$ annealed at 450 °C for 6 h exhibited the RTFM with high saturation magnetization of 4.91×10^{-3} emu/g for the $Sn_{0.92}Cr_{0.04}Mn_{0.04}O_2$. The origin of observed RTFM in the annealed samples was related to the defects based bound magnetic polaron model.

k0032

Structural And Magnetic Properties Of a New High-T_c Heusler Alloy Rh_2FeAl

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In this work we report a new Heusler compound Rh_2FeAl. XRD analysis confirms presence of B2 type of disorder, while magnetization study reveals high temperature magnetic ordering. Isothermal magnetization study shows the deviation of saturation moment from the

theoretically predicted Slater-Pauli value indicating the presence of structural disorder in the system.

k0033

Structural and magnetic properties of a new quaternary Heusler alloy CoFeVAl

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Powder X-ray diffraction and magnetic measurement for a novel quaternary Heusler alloy CoFeVAl reported for the first time. The single-phase and quaternary Heusler alloy structure of the compound established from diffraction pattern taken at room temperature. Temperature dependence of magnetization and isothermal magnetization measured at 2 K reveal the magnetic transition temperature and saturation magnetization to be 58 K and 0.58 μ_B/f.u., respectively.

k0035

Transient Reflectance Ultrafast Spectroscopy (TRUS) in PLD grown $Y_3Fe_5O_{12}/Gd_3Ga_5O_{12}$

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Magnetization dynamics control at picosecond timescale is of great technological importance from research as well as industrial perspective. In this report we present a detailed study on structural as well as transient ultrafast spectroscopy study on PLD grown YIG thin films. The HRXRD study reveals the growth of film epitaxially on GGG <110> and the XRR study confirms the thickness and quality of the deposited film. Further, high crystallinity is defined by very narrow FWHM values of 0.0047^O for YIG obtained from the ω scan. To study the ultrafast photomagnonic phenomena we excited the film with 2.81eV (440nm) pump energy at a different average power and recorded the differential reflectance through pump-probe method. This study develops a link between photonics and magnonics and results in generation of terahertz frequency from a room temperature ferrimagnetic garnet YIG.

k0037

Impedance Spectroscopy Of Metamagnetic Eu_2CoMnO_6

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We report on impedance spectroscopy of polycrystalline Eu2CoMnO6. The structural analysis shows that the Eu_2CoMnO_6 crystallized in a single orthorhombic phase. The cole-cole plot shows single semicircle. The analysis of cole-cole plot and imaginary part of impedance shows semiconducting nature of Eu2CoMnO6. The real part of impedance shows a high value at low temperature and frequency while it decreases at higher temperature and frequency due to increased mobility of charge carrier at higher temperature.

k0038

Magnetic Property Of Double Perovskite EuPrCoMnO6

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We report on structural and magnetic study of polycrystalline EuPrCoMnO6. The structural analysis shows that the EuPrCoMnO6 crystallized in a single orthorhombic phase with a space group Pnma. The temperature dependent magnetic study shows multiple magnetic transition below 160 K. The bifurcation between ZFC/FC magnetization curve shows presence of spin frustration in system. Inverse DC susceptibility shows presence of clustered phase in paramagnetic matrix.

k0039
Magnetic and Magnetocaloric Properties of Polycrystalline Bulk and Nanocrystalline $Sm_{0.5}Ca_{0.15}Sr_{0.35}MnO_3$ Compound
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The magnetic and magnetocaloric properties of $Sm_{0.5}Ca_{0.15}Sr_{0.35}MnO_3$ compound reveals that the disordered ferromagnetic and charge ordered antiferromagnetic counterparts present in bulk sample are drastically modified in its nanocrystalline form. The signature of the inverse magnetocaloric part (arises due to kinetically arrested antiferromagnetic phase) at low temperature is vanished with the development of the ferromagnetic correlation in nanocrystalline form of the sample.

k0040
Longitudinal Spin Seebeck Effect on $Li_{1.02}Fe_5O_8$
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Longitudinal spin Seebeck effect (LSSE) refers to the generation of pure spin current parallel to applied temperature gradient in a magnetic material. In this paper we report LSSE measurements on inverse spinel lithium ferrite compound $Li_{1.02}Fe_5O_8$ having ferrimagnetic structure (determined using the neutron diffraction technique). The LSSE measurement were performed using the indigenously developed LSSE measurement setup. The observed LSSE voltage (V_{ISHE}) depends on the direction of external magnetic field, following the relation $E_{ISHE} = (\theta_{SH}\rho)J_S x\sigma$ where J_s and σ are spin current density and spin polarization vector, respectively.

k0041
Emergence of Magnetic Moment by Doping of 3d Transition Dopant in BeP_2 Monolayer
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In this work, we have reported the nature of BeP_2 monolayer by doping of 3d, 4d and 5d transition metal atom with replacing single atom of Be and P atom in the super cell of BeP_2 monolayer. We have focused on magnetic properties of BeP_2 monolayer using density functional theory. As we found that 3d transition metals (Fe, Co and Ni) are good candidate for emerging magnetic moment in the system. The pristine BeP_2 monolayer behaves as non-magnetic system with Dirac code at Fermi level. There are few previous reported works, who declare the stability of pristine BeP_2 monolayer. The magnetic moments for Fe (Be+P), Co (Be+P) and Ni (Be) doped to BeP_2 monolayer as 2.96, 3.04, 1.65, 1.41 and 1.07 μB, respectively. This doped systems could be used for a spin diode.

k0042

Magnetic Properties of Triangular Lattice Pr_2NiGe_3

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Ternary intermetallic compound Pr_2NiGe_3 has been synthesized by arc melting technique and characterized by X-ray diffraction and dc magnetization measurements. The compound crystalizes in hexagonal crystal structure with space group *P6/mmm* where the rare earth atoms are arranged in 2-dimentional triangular lattice along the c-direction. Magnetic study reveals a magnetic ordering near 12.8 K and an additional phase transition around 3.2 K. The non-saturating nature of isothermal magnetization, along with the positive but low value of paramagnetic Curie temperature (θ_p ~ 1.2 K) suggest the antiferromagnetic ordering in association of dominating ferromagnetic interaction. The low temperature anomaly at 3.2 K could thus be attributed to the glassy nature of the magnetic spins due to the simultaneous presence of both the antiferromagnetic as well as ferromagnetic interaction.

k0043

Evidence for octahedral tilting in antiferromagnetic La_2TiCoO_6

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Transition metals based double perovskite: La_2TiCoO_6 was synthesized using standard ceramic method. X-ray characterization showed that this compound exhibited monoclinic structure, space group $P2_1/n$ with two formula units per unit cell. Ordering of Ti and Co ions in rock-salt arrangement over B-sites was confirmed by the observation of super lattice reflections. Various structural parameters, bond lengths and angles were extracted from Rietveld refinement analysis. Small distortion index calculated for cobalt octahedra suggested high spin state for divalent cobalt ion. Octahedral tilt estimated from refinement is found to be ~12°. Magnetic transition around 12.5 K was observed in temperature dependent magnetization data and is ascribed to antiferromagnetic transition as inferred from the Curie temperature.

k0044

Formation of Nickel Silicide and Appearance of Anomalous behaviour of Magnetic Anisotropy in Nickel thin films

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In the present work, we have study the formation of nickel silicide at the interface of nickel and silicon (Si), when the nickel (~15nm) is deposited on Si substrate (Si/Ni). Further, we have determined formation of different phases of nickel silicide with temperature annealing by using X-ray reflective (XRR). Besides this, we have investigated the magnetic properties, i.e. magnetic anisotropy and magnetic domain microstructure of as-deposited nickel thin film. For the sake of comparison of interface effect and magnetic properties, we have deposited another Ni film with a buffer layer of Pt between the nickel and Si substrate (Ni/Pt/Si), and examine its magnetic and structural properties. It is found that Si /Pt /Ni is textured along (111) direction, and it has no magnetic anisotropy. However, for Ni/Si, we observed anomalous magnetic anisotropy behaviour (referred to as the collapse of hard axes), i.e., anomalous behaviour of magnetic reversal process at hard axes of magnetization due to magnetic dispersion.

k0045
Superconductivity in layered Quasi-1D $Ta_2Pd_{1-\square}S_5$ nanostrips
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Topological superconductors with Majorana bound states obey non-Abelian statistics that are potential candidate for quantum computation. Correlated Quasi-1D electron gas systems are known to exhibit most commonly hidden order transition Charge/Spin Density Wave (CDW/SDW) and few predictions of topological aspects. Hidden order transitions are class of slow dynamics and show strong spectroscopic signatures in conductance noise spectroscopy. Here we report the synthesis and characterization of $Ta_2Pd_{1-\square}S_5$ ($\square$~0.13) which is a Quasi-1D system. Electronic transport of TPS is insulating in nature and metallic state appears with anomaly in resistivity below 5 K. Deficiency of Pd cites leads to such phenomena

k0046
Temperature Dependent Magnetic Studies of Ni-Zn Ferrites Synthesized by Polyol Method
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The effect of Nickel substitution in Zinc ferrite powder is investigated. A series of $Ni_xZn_{1-x}Fe_2O_4$ nanocrystalline powder ($Ni_xZn_{1-x}Fe_2O_4$, x = 1, 0.75, 0.5, 0.25,0) were prepared by Polyol method and annealed at 800^0C for 12 hours. The samples were then characterized using X ray diffraction as well as Vibrating sample magnetometry (VSM). The temperature dependent magnetic properties were also studied. XRD results revealed that the prepared samples were of Cubic spinel structure and particle size falls in nano meter range. The magnetic hysteresis at room temperature and 5K was recorded. The saturation magnetisation increases gradually from X = 0.0 to 0.5 and reaches to the maximum value and then decreases gradually while Ni^{2+} composition increases. The coercivity, retentivity and its variation with Nickel concentration are studied in detail. The

temperature dependent magnetic studies predicted the superparamagnetic behaviour of the samples.

k0047

Clustered Phase and Meta-magnetic Transition in $EuTbMnO_6$

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We report on structural and magnetic property of polycrystalline $EuTbCoMnO_6$. The structural analysis shows that $EuTbCoMnO_6$ has single orthorhombic phase with space group Pnma. Temperature dependent magnetization study shows a ferro-mgnetic magnetic transition around 113 K. The inverse DC susceptibility shows a down-turn, showing emergence of clustered phase in para-magnetic matrix. The bifurcation between ZFC/FC shows existence of spin frustration in the system

k0050

Topological Insulating Phase In Two-Dimensional Selenene Sulphide: A DFT Study

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We use Density Functional Theory based *first-principles* method to investigate Topological Insulating phase in two dimensional selenene sulphide. The sulphur functionalization of selenene gives rise to dynamic stability since, selenene independently cannot exist in hexagonal lattice due to its electronic configuration. This also gives rise to orbital filtering effects leading to non-trivial topology owing to the broken spatial inversion symmetry. Such non-trivial characters are attributed to the spin-orbit coupling effects which opens a band gap of $\Delta E = 0.167$ eV. We further analyze the non-trivial topology in terms of the $\mathbb{Z}_2$ invariant and the robust edge states which exhibits chiral spin polarization; confirming the quantum spin Hall effect. This indicates that, Selenene Sulphide has potential room temperature spintronic and nanoelectronic applications.

k0051

Magnetic And Transport Properties Of $Co_2V_{1.4}Ga_{0.6}$ Shape Memory Alloy

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In this work, we have observed a martensitic like structural transition that occurs between paramagnetic(PM) austenite and PM martensitic phases in the studied $Co_2V_{1.4}Ga_{0.6}$ alloy. Their might be a ferrimagnetic state present at temperature below about 50 K. Slight deviation of V concentration from $Co_{50}V_{34}Ga_{16}$ leads to drastic drop in magnetisation value and magnetic transition temperature. The magnetic behaviour observed in the $Co_2V_{1.4}Ga_{0.6}$ is quite different from those of previously reported conventional Ni-Mn based ferromagnetic shape memory alloys

k0052

Observation of the Griffith like phase in $Pr_2CoFe_{0.5}Mn_{0.5}O_6$

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$Pr_2CoFe_{0.5}Mn_{0.5}O_6$ (PCFMO) system is prepared which is crystallized in orthorhombic phase with Pnma space group. The dc magnetization indicates the magnetic transition at 187 K whereas the Curie Weiss (CW) fit reveals the dominating ferromagnetic (FM) interaction in the system. Moreover, the $1/\chi$ shows the typical downturn behaviour which is the symbol of the presence of Griffith phase in present system.

k0053

Preparation And Characterizations Of Gallium Substituted X-type Strontium Hexaferrites

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Ferrites are ferromagnetic ceramic oxides. The structural and magnetic properties can be tuned by amount and size of substituted cations, heating temperature and heating time as well as cooling rate. Gallium substituted X- type hexaferrites were synthesized using citrate gel auto combustion method. Prepared samples were characterized using FTIR, XRD and VSM. The XRD analysis shows formation of X, along with W and M phases. The high saturation magnetization ~91 A m^2 kg^{-1} is observed for the sample prepared without gallium and substituted samples show variation of saturation magnetization from 90 A m^2 kg^{-1} to 65 A m^2 kg^{-1}. Very low values of M_r/M_s suggest the multi domain nature of the particles.

k0054

Structural and dielectric study of solid state prepared double perovskite Tb_2NiMnO_6

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Phase pure double perovskite Tb_2NiMnO_6 (TNMO) have been prepared by employing solid state reaction method. The earlier study on TNMO reported presence of secondary phase. The prepared sample was subjected to X- Ray diffraction (XRD) and neutron diffraction (ND) at ambient temperature. The analysis by Rietveld refinement confirmed the phase purity. The sample was found to crystallize in the monoclinic structure with $P2_1/n$ space group (sg # 14). The dielectric constant as a function of frequency at room temperature was also studied. In order to identify and study the contribution due to different effects, present in the sample, the Cole-Cole plot have been derived from the data and two semi-circles are evident which is indicating the presence of grain and grain boundary in the sample. We are in process of studying the SEM to ascertain the observation pertaining to grain and grain boundary.

k0055

Quantitative Interdependence Of Spin Spirality And Electric Polarization In $CoCr_{2-x}Fe_xO_4$ Spinel Compounds

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Quantitative interdependence of spin spirality and electric polarization has been probed in $CoCr_{2-x}Fe_xO_4$ spinel compounds. These compounds undergo spiral ordering (T_S) and concomitant electric polarization below ~25 K. The T_S is seen decreasing with more Fe (x)

substitution as observed from dc magnetization measurements. Neutron diffraction study has inferred a decrease in spirality of both *A* and *B*-sites spins with increasing the *x*. Electric polarization study, on the other hand, has suggested an increase in polarization with increasing substitution of Fe, thus revealing a direct correlation between spin spirality and electric polarization.

k0056

Evidence of Temperature-Dependent Magnetodielectric Effect in $KBiFe_{1.9}Co_{0.1}O_5$

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Single-phase Cobalt (Co) doped $KBiFe_2O_5$ ($KBiFe_{1.9}Co_{0.1}O_5$: KBFCO) is prepared by conventional solid-state reaction route. Rietveld refinement of X-ray diffraction data confirms the single phase of KBFCO and crystallizes in monoclinic structure with *P2/c* space group. Surface morphology characterization reveals the grains are randomly distributed, and the average grain size formed is in the range of ~1-5 μm. The temperature (10 K to 300 K) and frequency (500 Hz to 1 MHz) dependent dielectric permittivity value decreases approximately 50% in the presence of a 1.3 T magnetic field. Our result confirms a sizeable magnetodielectric (MD) effect (MD% ≈ -50% near Room Temperature) in the entire measured temperature range. The measured MD effect is recorded at the high-frequency (20 kHz to 1 MHz) range, suggesting the intrinsic effect is dominated in the probing temperature range. These results confirm that KBFCO has an excellent MD response even for a small applied field.

k0058

Magnetization Reversal and Exchange-Bias in Highly Anisotropic Ferrimagnetic Compound, $DyFe_5Al_7$

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Intermetallic compound, $DyFe_5Al_7$ has been prepared by arc melting method. X-ray diffraction infers the single phase formation of the compound. DC magnetization under 50 Oe reveals that ferrimagnetic ordering sets in the compound at ~ 235 K (T_C) and magnetization reversal phenomenon below T_{COMP} (~ 93 K). Moreover, the compound shows the exchange bias phenomenon below ~ 50 K. A giant exchange-bias as well as and coercivity with values of ~ 2 kOe and 18.3 kOe (5 K), respectively are observed.

k0060

Effect of Isothermal annealing on the magnetic property of Carbon thin film

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The effect of isothermal vacuum annealing on the microstructure and magnetic property of amorphous carbon thin deposited using RF magnetron sputtering at RF power of 150W is

discussed. The as-deposited film consists of both superparamagnetic and paramagnetic sites distributed throughout the film. Microstructure characterization studied using Raman spectroscopy (RS) confirms that the rehybridization of sp^3 to sp^2 bonded atoms prevails on annealing. The X-ray Reflectivity (XRR) measurement reveals that the bulk density decreases considerably with annealing temperature. The magnetic measurement indicates that the paramagnetic sites are extinct on annealing, whereas the bulk saturation magnetization of the film decreases considerably. The effect of thermal annealing on the hybridization ratio and its consequence on the amorphous carbon thin film's magnetic property is explained.

k0061

Evidence of Magnetodielectric Coupling in (1-x)$Bi_5Ti_3FeO_{15}$-(x)$La_{0.67}Sr_{0.33}MnO_3$ (x= 0.0 and 0.1) Composites

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Composite (1-x)BTFO-(x)LSMO (x= 0.0 and 0.1) is synthesized by sol-gel modified technique in order to study the magnetodielectric (MD) properties. Rietveld refinement of the X-ray diffraction (XRD) patterns confirm the existence of dual-phases orthorhombic ($A2_1am$) and rhombohedral ($R\text{-}3c$) in the composites. The systematic change in dielectric permittivity with a static magnetic field (0 T and 1.3 T) indicates the signature of the MD effect in the composite. The magnitude of the room temperature the MD effect is 0.08% for x= 0.1 composite, which is twenty times higher than that of the x= 0.0 sample with 0.004% at 1.3 T field.

k0062

Interfacial Spin Scattering Enhanced Magnetoresistance in $La_{0.7}Sr_{0.3}MnO_3$/ZnO Heterostructures Integrated on (001) Si

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A series of $La_{0.7}Sr_{0.3}MnO_3$(LSMO)/ZnO heterostructures with different ZnO thicknesses were grown on (001) oriented Si substrate at 700 °C using RF magnetron sputtering. The X-ray diffraction patterns indicate the (00l) orientation of LSMO and ZnO films. The LSMO thin film shows positive as well as negative magnetoresistance (MR). The charge transfer induced interfacial antiferromagnetic coupling at the Si-LSMO interface and spin-orbit coupling due to the presence of non-collinear Mn ions spins at the interfaces and surfaces are responsible for the positive MR of LSMO thin film. However, the positive MR is suppressed and negative MR is enhanced by depositing a ZnO film on the Si/LSMO. The out-of-plane negative MR of LSMO/ZnO heterostructures increases with ZnO thickness. This type of MR behavior of LSMO thin film and LSMO/ZnO heterostructures integrated on Si can be used in spintronic applications.

k0064

Magnetization Reversal in Double Perovskite Y_2FeCrO_6 Nanoparticles

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Here we have opted gel combustion route to prepare single phase nanoparticles of Y_2FeCrO_6 (YFCO) sample and reported its structural and magnetic behavior. According to the room temperature XRD and Raman spectra analysis the sample comes under monoclinic phase with $P2_1/n$ space group. The average particle size as per microstructural image is 67 nm. Magnetization versus temperature (M-T) analysis reveals that the material exhibits negative magnetization below 143 K (T_{comp}). Magnetization versus field measurement (M-H) at 5 K indicates presence of mixed magnetic phase in the sample.

k0065

Synthesis and Characterization of Topological Superconductor $SnTaS_2$

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We have studied the superconducting properties of dichalcogenide compound $SnTaS_2$. We have grown single crystals using Chemical Vapor Transport (CVT) method. The single crystal structure was confirmed by XRD pattern of flake, which consists only (0 0 *l*) peaks. Critical temperature T_c was found to be 2.8K. Magnetization study indicates signature of type-II superconductor.

k0066

Impact of Heating Temperature on Structural and Dielectric Properties of Magnesium Ferrites

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The spinel $MgFe_2O_4$ ferrites were synthesized using sol-gel auto-combustion technique and heated at 650 ℃, 750 °C and 1050 °C for 4h. X-ray diffraction (XRD) and low frequency dielectric measurements are used to characterize $MgFe_2O_4$ ferrite. XRD analysis of samples heated at 750 °C and 1050 °C show pure spinel phase while the sample heated at 650 °C revealed formation of spinel with hematite. Dielectric study of all samples was carried out in the frequency lies between 100Hz-2MHz. Dielectric measurements show frequency dependant phenomena. Dielectric constant found to decrease with frequency.

k0067

Effect of Excessive Mn Doping on Electrical Properties of Skyrmionic MnSi

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We report here on the synthesis and zero-field electrical resistivity measurements on the confirmed skyrmionic compound MnSi. Polycrystalline MnSi sample has been prepared through arc melting process. The phase purity and the crystal structure of the sample has been analyzed using Rietveld analysis and a secondary phase of Mn_5Si_3 is identified. Temperature dependence of resistivity shows a drop around Tc ~27.5 K which is indicative of the onset of

magnetic ordering. Evidence for the dominance of electron-electron scattering mechanism in the ferromagnetic phase is provided.

k0068

Effect of Mg^{2+} Substitution on Structural and Magnetic Properties of W-type Strontium Zinc Hexaferrites

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Mg- substituted W-type hexaferrites with chemical composition $SrZn_2Mg_xFe_{16-x}O_{27}$ (x = 0.0, 0.2, 0.4, 0.6, 0.8, 1.0) were synthesized using sol-gel auto combustion method, and subsequently heated at 1300 °C for 5 h. The structural and Magnetic properties of prepared hexaferrites were investigated using FTIR, XRD and VSM techniques. The FTIR analysis of all samples shows two absorption bands between wave-number ranges of 600-400 cm^{-1}. The XRD analysis of the sample x = 0.0 shows formation of pure W-type phase, while other Mg-substituted samples show W-type phase along with M-phase. VSM analysis of all samples shows that formed samples possess soft magnetic nature having multi-domain structure.

k0069

Linear And Non Linear Optical Properties of $Bi_{0.95}Sr_{0.05}Fe_{0.95}Mn_{0.05}O_3$ Ceramic

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In this study, $Bi_{0.95}Sr_{0.05}Fe_{0.95}Mn_{0.05}O_3$ ceramic sample was synthesized by conventional Solid state reaction. Third-order nonlinearity of multiferroic ceramic was studied by Z-Scan technique in which nonlinear absorption coefficient **(β)** was evaluated by the open aperture Z-Scan technique using continuous wave (CW) laser of 405nm wavelength. Prepared ceramics shows reverse saturation absorption (RSA) behaviour. XRD reveals the single-phase rhombohedral structure with R3c space group. Optical properties like absorption band, band gap and linear refractive index were analysed by UV-Visible spectroscopy. Morphology of the sample was analyzed by FESEM, represents the homogeneous agglomerated particles.

k0070

Study of Structure, Dielectric, and Magnetodielectric Properties of Polycrystalline $KBi_{0.95}Ho_{0.05}Fe_2O_5$

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Holmium modified polycrystalline KBiFe2O5 (KBi0.95Ho0.05Fe2O5) having a P2/c space group is synthesized using a solid-state reaction route. The phase purity is characterized by X-ray diffraction measurement. The temperature-dependent dielectric permittivity is

analyzed over a wide temperature range (10 K to 300 K) in the presence of 1.3 T and 0 T magnetic fields. The shifting of temperature-dependent dielectric permittivity (ε′) with the magnetic field indicates the magnetodielectric (MD) signature. Variation of MD with magnetic field shows a butterfly-like MD loop. The extracted maximum room temperature magnetodielectric coupling is found to be 0.2% in KBi0.95Ho0.05Fe2O5. These results made it a prominent candidate for multifunctional device applications and provided space to investigate further the microscopic origin behind it.

k0072

SQUID Based Magnetocardiographic Mapping Of Fragmented QRS Activity In A Cardiac Cycle Using Sample Entropy

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The term "fragmented QRS" (fQRS) refers to one or more deflections within the normal duration of the QRS complex (<120 ms). fQRS is induced by conduction abnormalities in the cardiac tissue or due to the presence of scar tissue subsequent to myocardial infarction (MI). Magnetocardiography (MCG) is a non-contact, non-invasive method to probe the electrophysiology of the heart by measuring its magnetic signals. MCG is effective in localizing myocardial areas where fragmentation occurs. Sample entropy (SE) measures the regularity or repeatability of a pattern in the time series. Fragmentation score (FS) gives a value based on the number of extrema present. The current work estimates SE and FS on the QRS complexes for a subject with an old inferior MI and for a healthy control subject. The acquired parameters are utilized to build two dimensional (2D) spatio-temporal contour maps, which hints at the possible areas of myocardial infarct. This preliminary finding implies that SE could be a useful biomarker in post MI assessments.

k0074

Anomalous Magnetization and Magnetocaloric Effect of $Co_2TiAl_{1-x}Si_x$ Full Heusler Alloys

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The half-metallic ferromagnets Co_2TiZ (Z= main group element) show tunable transport properties, high Curie temperatures, and high magnetic moments. The present $Co_2TiAl_{1-x}Si_x$ (x=0.50, 0.75) alloys have been prepared by the conventional Arc melting technique and their magnetic properties have been analyzed. These alloys exhibit a wide range of transition temperatures from 285 K to 315 K near room temperature and theoretical magnetic moment between 1.50 μB/f.u. to 1.75 μB/f.u. with increasing Si concentration. However, experimentally it is observed that the saturation magnetization for x=0.75 slightly deviates from Slater Pauling's prediction. Also, the magnetocaloric effect study of this series reveals that these materials (specially x=0.50) can be tuned for magnetocaloric application near room temperature.

k0076

Magnetic and magnetocaloric properties in Al doped Ni-Co-Mn-Sn-based Heusler alloy

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Herein, the tuning of martensitic transformation and the magnetocaloric properties are investigated for the $Ni_{44}Co_3Mn_{38}Sn_{14}Al_1$ Heusler alloy. The alloy shows austenite phase corresponding to $L2_1$ cubic structure at room temperature. From magnetic measurement, the sample is found to undergo a first-order martensitic transformation (MT) from a ferromagnetic austenite phase to a weak magnetic martensitic phase. A maximum value of isothermal magnetic entropy changes of about 5 $Jkg^{-1}K^{-1}$ associated with a relative cooling power of ~137 Jkg-1 is obtained due to field change of 5T. The material shows the large magnetocaloric response in a wide working temperature interval of 27 K which will lead this alloy as a potential magnetic refrigerant material for magnetic refrigeration.

k0077
Structure Mobilized Magnetic Transitions in Ca Doped $Y_{2-x}Ca_xRu_2O_7$
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In summary, we report on an experimental investigation of the structural and magnetic properties of the $Y_{2-x}Ca_xRu_2O_7$ pyrochlore system as a function of Ca doping in the range $0.00 \leq x \leq 0.4$. The structural properties show the presence of lattice expansion in the crystal structure, which we have verified from the Rietveld data of the XRD pattern. The temperature dependence dc magnetic susceptibility data shows the Curie-Weiss constant (θ_C) and the frustration parameter (θ_C/T_N) decreases systematically with the Ca concentration, which suggests Ca-doping promotes release of magnetic frustration in YRO. The transition of Neel temperature towards the lower side suppresses the glassy behavior which is caused by the increase of the itinerant carriers in the system. We see a decrement of effective moment with increasing x at the ruthenium site, which indicates the presence of Ru^{5+} ion in D_{3d} symmetry or the hybrid Ru^{4+}/Ru^{5+} ion in the sample after doping a divalent atom in the position of trivalent atom.

k0078
Large magnetocaloric effect in $Ho_{15}Si_9C$
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The ground state magnetic properties and magnetocaloric effect (MCE) of $Ho_{15}Si_9C$ compound isostructural with $R_{15}Si_9C$ (R = Gd, Tb, and Dy) are investigated. $Gd_{15}Si_9C$, $Tb_{15}Si_9C$, $Dy_{15}Si_9C$, and $Ho_{15}Si_9C$ exhibit second order ferromagnetic transitions at temperatures below 170 K, 130 K, 70 K, and 42 K, respectively. For $Ho_{15}Si_9C$, the maximum value of $-\Delta S_M$ is 11.04 J/kg K at 68 K for H = 50 kOe. The key finding of this research is that as the atomic number increases, the transition temperature of $R_{15}Si_9C$ (R = Gd, Tb, Dy, and Ho) decreases while the maximum entropy value rises. $R_{15}Si_9C$ compounds has high reversible MCE values, it could be useful for magnetic refrigeration. The presence of large MCE values is due to the large magnetic moment associated with rare earth elements.

k0080

Quasi-Two-Dimensional Magnetism in Spin-1/2 Square Lattice Compound $Cu[C_6H_2(COO)_4][H_3N\text{-}(CH_2)_2\text{-}NH3]\cdot 3H_2O$

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We have synthesized the single crystal of quasi-two-dimensional S = 1/2 quantum magnet $Cu[C_6H_2(COO)_4][H_3N\text{-}(CH_2)_2\text{-}NH_3].3H_2O$ and solved it structure and Investigated magnetic properties. It crystallizes in a monoclinic structure with space group $C_{2/m}$. The CuO_4 plaquettes are connected into a two-dimensional framework in the *ab*-plane through the anions of $[C_6H_2(COO)_4]^{4-}$ (pyromellitic acid). The $[H_3N\text{-}(CH_2)_2\text{-}NH_3]^{2+}.3H_2O$ groups are located between the two adjacent layers and provide a weak interlayer connection via hydrogen (H...O) bonds. The temperature dependent molar magnetic susceptibility is well described by S = 1/2 frustrated square lattice ($J_1 - J_2$) model with nearest-neighbor interaction $J_1/k_B \simeq 5.37$ K and next-nearest-neighbor interaction $J_2/k_B \simeq -0.37$ K. Our analysis using frustrated rectangular lattice ($J_{1a,b} - J_2$) model also confirms almost isotropic nearest-neighbour interactions ($J_{1a}/k_B \simeq 5.31$K and $J_{1b}/k_B \simeq 5.38$K) in the *ab*-plane and $J_2/k_B \simeq -0.24$ K. Further, the molar susceptibility at $\mu_0 H = 0.5$ T and the isothermal magnetization at $T = 1.9$ K is also well described by a non-frustrated square lattice model with $J_1/k_B \simeq 5.2$ K. Based on the J_2/J_1 ratio, the compound can be placed in the N´eel antiferromagnetic state of the $J_1 - J_2$ phase diagram. No signature of magnetic long-range order is detected down to 2 K.

k0081

Structural and Magnetic Properties of Hexagonal $BaMnO_3$

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Though the presence of short-range magnetic ordering and temperature induced structural transitions in $BaMnO_3$ have been reported by several studies but detail explanation on the magnetization of 2H-$BaMnO_3$ is controversial. In this work we report the debatable structural and magnetic features of nanosized hexagonal $BaMnO_3$ samples with $P6_3mc$ space group synthesized by ethylene derived sol-gel route under ambient atmospheric and low-temperature conditions. Magnetic susceptibility measurements carried out at low and high dc fields on the compound between 5K and 300 K were identified with the appearance of antiferromagnetic ordering around transition temperature of 50 K. On the other hand, non saturating magnetization value of M-H curve at higher applied field clearly suggests the small canting in AFM state of 2H-$BaMnO_3$ and at high temperature, M-H curves show linear behavior.

k0082

Study on Structural, Magnetic and Exchange Bias Properties of Mn-Ni-Co-Sn Heusler Alloy

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Here, we have investigated the structural, magnetic, and exchange bias properties of a Mn rich $Mn_{50}Ni_{42-x}Co_xSn_8$ (x=6) Heusler alloy. Present alloy undergoes the magneto-structural (martensitic) transition at around 333 K, and the low temperature magnetic state of the alloy has been investigated by means of DC magnetization and AC susceptibility measurements. These measurements confirm the presence of spin glass (SG) phase at low temperatures. A large exchange bias field of 990 Oe is observed after field cooling the alloy at 10 kOe field. This is attributed to the large exchange anisotropy present at SG/FM interfaces. The temperature and cooling field effect on the exchange bias properties has also been studied in this report.

k0083

Study of Pseudogap in YBCO:$NaNbO_3$ Nanocomposite Thin Films

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In high temperature superconductors, the short coherence length and charge carrier concentrations are responsible for the thermal fluctuations in the resistivity curve. The effect of $NaNbO_3$ nanoparticles and nanorods addition on the basal-plane conductivity of YBCO thin films has been investigated. Thin films of pure YBCO and YBCO:$NaNbO_3$ composites have been deposited on $SrTiO_3$ substrate using pulsed laser deposition (PLD) technique. The growth of c-axis orientation is confirmed in pure YBCO and YBCO:$NaNbO_3$ thin films using the structural analysis. In the thermal fluctuations regime, the excess conductivity shows exponential dependence on temperature which is used to obtain information of pseudogap at temperatures away from critical temperature T_C. The characteristic temperature have been found higher for the Nanocomposite thin films than the pure YBCO thin film, which indicates the extended excess conductivity region.

k0084

Study of Magnetic Behaviour of Mg-Mn-Zn ferrites using Mössbauer Spectroscopic Technique

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In the present manuscript structural and Mössbauer results of $Mg_xMn_{0.8-x}Zn_{0.2}Fe_2O_4$ (x = 0.1, 0.4, 0.7) nanoferrites are reported. XRD patterns revealed the formation of spinel phase along with anti-ferromagnetic phase of α-Fe_2O_3. Both lattice parameter and crystallite size is decreasing with the substitution of Mg^{2+} ions. Mössbauer spectra consist of fully resolved six line patterns along with quadruple dublets. The isomer shift values are the indicative for the existence of Fe^{3+} ions only. The higher value of line width of octahedral (B) site revealed the core-shell morphology of ferrite nanoparticles showing spin-glassy interactions. It is

supported by marginal variation of hyperfine field (H_f) of tetrahedral (A) and octahedral (B) sites. The present series of ferrite samples are useful for multifunctional applications due to presence of fine ferrite nanoparticles.

k0085

Ultrasonically assisted wet-chemical synthesis of Lu doped $BiFeO_3$

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Lu doped $BiFeO_3$ (BFO) was successfully prepared via a wet-chemical route with assistance from high power ultrasound (150W). The synthesis process was further hastened by utilizing the power of uniform microwave heating. X-ray powder diffraction data and Rietveld refinements of XRD data revealed that the phase formed compound has a rhombohedral structure with R3c space symmetry. A minor secondary phase was identified as $Bi_2Fe_4O_9$ in the range between 2θ~(25°-30°), which usually occurs while synthesizing BFO.

k0086

Structural Study of Samarium and Gallium Co-Doped Multiferroic Bismuth Ferrite

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Samarium (Sm) and (Gallium) Ga co-doped on A and B-site of Bismuth Ferrite ($BiFeO_3$ or BFO) sample was synthesized using solid state reaction method by quenching technique. This is then followed by investigations into the influence of Sm and Ga co-doping on the structural and morphological properties of $Bi_{0.95}Sm_{0.05}Fe_{0.975}Ga_{0.025}O_3$ using XRD, Rietveld refinement and SEM with EDS. X-ray diffraction analysis reveals the crystalline structure of doped BFO and its phase formations. The Rietveld refinement reveals that the A and B-site co-doping of Sm and Ga lead to the transformation of its crystal structure from a rhombohedral with a space group of *R3c* to an orthorhombic with a space group of *Pbam*. The phase fraction of 69 % was obtained for the BSFG and the rest was converted into its secondary phase $Bi_2Fe_4O_9$. The Field Emission Scanning electron microscope (FESEM) image and EDS study depicts the grain size and elemental composition of the sample.

k0087

Intrinsic Room Temperature Ferromagnetism in van der Waals Fe_5GeTe_2 Crystal

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Two dimensional magnetic materials have drawn a great attention in 2D magnetism and opened up a new direction for modern spintronic applications. Here, we have synthesized a cleavable Fe_5GeTe_2 material, which shows an intrinsic ferromagnetic behaviour at room temperature (~310K). We have investigated the electronic and magnetic properties of the bulk Fe_5GeTe_2 single crystal. Our study reveals that bulk Fe_5GeTe_2 is metallic and behaves like an easy-axis ferromagnet along c-axis with a stronger in-plane magnetic anisotropy compared to the out of plane. However, the magnetic state of Fe_5GeTe_2 is much complex and still unclear, hence systematic investigation may lead this material as an ideal candidate for spintronic applications.

k0088

Low-temperature magnetotransport studies on $Nd_{0.6}Sr_{0.4}MnO_3$ thin films

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Magnetotransport measurements performed on $Nd_{0.6}Sr_{0.4}MnO_3$ thin films having an insulator-metal transition at ~110 K reveal an upturn in its resistance in the low-temperature regime. A suppression in this resistive upturn upon application of magnetic field was observed. Further analysis using the low-temperature transport model indicates that grain-boundary or domain wall scattering, Kondo-like scattering, and strong correlation effect contribute significantly to this resistive upturn.

k0090

Superconductivity in Ir doped $LaRu_3Si_2$ Kagome superconductor

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In this report, we investigated the impurity induced effects on the superconducting properties of the Kagome lattice system $LaRu_3Si_2$. Initially, the phase purity and the crystal structure of prepared $La(Ru_{1-x}Ir_x)_3Si_2$ (x = 0,0.05,0.1) samples were determined from room temperature powder x ray diffraction data. No noticeable peak shifting was observed for the Ir doped samples from Rietveld refinement data as the radius of Ru^{4+} is nearly comparable to the radius of Ir^{4+}. We performed a temperature dependent magnetization measurement and electrical resistivity measurement for the samples. Our results show a downward shift of the transition temperature with Ir(5d) doping concentration. The diamagnetic signal in the ordered state is close to the ideal magnitude of $-\frac{1}{4\pi}$ indicating the superconducting volume fraction of nearly 100% for all the studied samples. We also note that the rate of suppression of T_C is higher than that of Co doping while it is lower than that of Fe doping.

k0091

Large Magnetic Entropy Change in van der Waals $CrBr_3$ Single Crystal

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Atomically thin intrinsic magnetic van der Waals (vdW) systems open a new platform in nanoelectronics as well as in fundamental physics in recent years. We have investigated magnetic and magnetocaloric properties of $CrBr_3$ single crystal from magnetic measurement. $CrBr_3$, a vdW semiconductor, with out of plane magnetic easy axis shows T_c around 33K. A large magnetic entropy change of 9.3J/kg-K is observed in $CrBr_3$ for a field change of 7T close to transition temperature. This indicates that $CrBr_3$ can draw significant attention as a magnetic refrigerant for liquefaction of hydrogen in fuel industry.

k0092

Synthesis of Pr doped $BiFeO_3$ via Sonochemistry assisted sol-gel method

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Synthesis of Pr doped – $BiFeO_3$ (BPFO) is successfully conducted via a wet-chemical route with additional assistance from high power(150W) ultrasound. The prepared ceramic powder was calcined at 350°C for 3hours, this was taken for X-ray diffraction (XRD) for phase analysis. Rietveld refinement of XRD data is successfully carried out by selecting the R3c space group in Fullprof software. Rietveld refinement manifest's rhombohedral structure with R3c group along with the existence of a secondary phase $Bi_2Fe_4O_9$. A reduction in synthesis time and temperature using this method is reported here.

k0093

Soft point contact Andreev Reflection spectroscopy to probe superconducting proximity effect in Nb thin films

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We report the use of soft point contact Andreev reflection spectroscopy (SPCAR) to probe superconducting proximity effect (SPE) in Nb thin films. SPCAR was carried out on Nb films with different thickness with a piece of indium pressed on it. The spectra were analyzed using the BTK model which gave the measure of the strength of the interface barrier (Z) and the superconducting energy gap (□). Our results show that the superconducting proximity effect (SPE) in the Nb thin films resulting in a reduction of □ at the point contact is primarily affected by the interface barrier (Z), irrespective of thickness of the film. SPE becomes more pronounced for low Z contacts indicating that surface sensitive SPCAR technique can probe SPE also in films with thickness greater than the coherence length of Nb.

k0094

Magnetocaloric Effect in $DyVO_3$

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The orthovanadate $DyVO_3$ has been synthesized by the solid-state reaction method. The material crystallizes in orthorhombic crystal structure at room temperature (space group *Pbnm*). Magnetic entropy change has been calculated from the isothermal magnetization measured in the magnetic field 0-5 T. At 2 K, the M-H isotherm tends to saturate with the increasing magnetic field. The maximum magnetic entropy change ($-\Delta S_M^{max}$) has been estimated to be 12.9 $Jkg^{-1}K^{-1}$ at an applied external magnetic field of 5T around 17K. The maximum entropy change occurs around the same temperature as that of the ordering of the Dy-sublattice.

k0095

Low-Temperature Magnetodielectric Effect in the $Nd_{0.5}Dy_{0.5}FeO_3$ Thin Film

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We have observed significant magnetodielectric effect in $Nd_{0.5}Dy_{0.5}FeO_3$ epitaxial thin film. The film is grown on $LaAlO_3$ (001) substrate by pulsed laser deposition technique. At 100 K, a variation of around 16% in dielectric constant is observed at frequencies higher than 2 MHz in the presence of 10 T and this variation in dielectric constant increases to about 50%

at 2 K. To utilize the observed magnetodielectric effect, we have designed a microstrip line based resonator with the help of High frequency simulation software (HFSS). Simulations are performed for the two values of dielectric constant (in the presence and absence of external magnetic field) to observe magnetic field tunability of the resonance frequency. A shift of 27% is observed in the resonant frequency of the microstrip line based resonator on $Nd_{0.5}Dy_{0.5}FeO_3$ epitaxial thin film.

k0096

Thermomagnetic studies on Te doped Dy_2O_3 for eco-friendly cryogenic magnetic refrigeration

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The work aims to investigate the magnetocaloric effect (an eco-friendly and energy-efficient cooling technique) of Te doped nanosized dysprosia, which could be used as the best alternative for conventional chlorofluorocarbons-based refrigeration systems. In this work, Te doped nanosized dysprosia (TNSD) was synthesized using the sol-gel technique. Samples showed anti-ferromagnetic (AFM) behaviour at low temperatures and paramagnetic (PM) at high temperatures. The maximum entropy change (ΔS_M) of TNSD at a magnetic field of 5 T was found to be 18 ~$JKg^{-1}K^{-1}$. The significant magnetic transitions at low temperature and large magnetic entropy change make TNSD suitable for eco-friendly cryogenic magnetic refrigeration.

k0097

Magnetic Field Dependent Photoresponse In P-type Si(100)/NiFe2O4/C60/ZnO-rGO Composite Heterostructure

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We studied light (660 nm) and magnetic field dependent current-voltage (I-V) characteristics of p-type Si(100)/$NiFe_2O_4$/C_{60}/ZnO-rGO composite heterostructure. Upon illumination of ZnO-rGO composite layer surface with 600 nm red light, photoresponse has been observed in the heterostructure. With the application of external magnetic field, current through the heterostructure is found to decrease both under dark and illumination. This decrease of current may be attributed to the positive magnetoresistance effect in the $NiFe_2O_4$ layer arising from the spin-dependent carrier transport through the layer. Coupled effect on the I-V characteristics of both light and external magnetic field has also been observed in our heterostructure.

k0099

Magnetic Properties of As-cast Half Heusler Compound CoCrAl

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Magnetic properties of polycrystalline as-cast half Heusler compound CoCrAl, prepared by arc melting, have been studied. A ferromagnetic to paramagnetic transition is observed near T_c =14 K though at 3 K non-saturating behavior is observed in field dependent magnetization (M-H) data even at 70 kOe applied magnetic field. It is found that the value of magnetization under 70 kOe field is 0.1μ_B/f.u. at 3 K. Magnetic clusters within paramagnetic matrix are found to be present because of Cr-Al disorder (B2 disorder) within the compound above T_c. Above 200 K, the inverse susceptibility as a function of temperature (χ^{-1}-T) curves at high magnetic field follows the modified Curie-Weiss law in which temperature dependent higher order Pauli paramagnetism term is included. Further analysis indicates that the state at low temperature can be considered as correlated cluster glass state.

k0100

Structural and dielectric properties of Tb and Mn codoped multiferroic $BiFeO_3$ ($Bi_{0.8}Tb_{0.2}Fe_{0.8}Mn_{0.2}O_3$)

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We have studied Tb and Mn codoping on crystal structure and dielectric properties of $BiFeO_3$ prepared via solid-state reaction method. There is the structural transition occur to orthorhombic (Pnma and $Pn2_1a$) phase from rhombohedral (R3c) phase. We have measured dielectric loss, and the dielectric constant (ε′) with temperature variation at different frequencies shows relaxor-type behavior.

k0101

Anti-ferromagnetic thickness dependent Exchange Bias and Domain Wall Dynamics in IrMn (t)/ Fe_2CoSi(5nm) Bilayers

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We report on the zero field cooled exchange bias (EB) and domain wall dynamics in IrMn (t)/Fe_2CoSi (5 nm) bilayers. We attribute the origin of EB to random domain configuration of IrMn (111) layer. Evolution of exchange bias is evidenced with the thicknesses of IrMn. The increase in exchange bias field (H_{EB}) above critical thickness ($t_{critical}$) of IrMn is explained on the basis of random field model in the Heisenberg regime. Indeed, there is perfect correlation between the bulk magnetization measurements and microscopic data obtained from longitudinal magneto optical Kerr effect (L – MOKE). These results suggest that IrMn (t)/Fe_2CoSi (5 nm) bilayers would indeed be useful in future spintronic device applications.

k0102

Magnetization switching effect due to flipping of Ce^{3+} moment in one step synthesized $CeCrO_3$

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Here, we have synthesized $CeCrO_3$ via a facile, fast, and cost-effective one-step solution combustion method using different fuels (citric acid, urea, and glycine). As prepared compound synthesized with citric acid shows amorphous $CeCrO_3$, and with urea, $CeCrO_3$ is formed with an additional phase of CeO_2 while with glycine pure phase $CeCrO_3$ are found. Magnetization vs. time measurement with varying magnetic fields demonstrate flipping of paramagnetic moment of Ce^{3+} in the direction of superposition field direction, of the internal field due to Cr^{3+} and external applied field. Such flipping of moment demonstrated bipolar magnetization switching in $CeCrO_3$ which makes these materials potential candidates for nonvolatile magnetic memory, magnetic switching, and spintronics devices.

k0103

Phenomenological Investigations on Magnetocaloric Properties of $La_{0.8}Bi_{0.05}Na_{0.15}MnO_3$.

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We report the structural, morphological and magnetocaloric properties of the Bismuth (Bi)-substituted manganite $La_{0.85-x}Bi_xNa_{0.15}MnO_3$ (x=0, 0.05). X-ray diffraction data implicates rhombohedral structure belonging to $R\bar{3}c$ centrosymmetric space group. The Bi_2O_3 added as substituent ensures densified compound even at low sintering temperature. The increase in grains size and decrease in magnetic transition temperature (T_C) are due to the Bi_2O_3 chemical potential. The phenomenological model is used to model the thermomagnetic behaviour of prepared samples. The sample with x=0.05 shows phenomenal increase in magnetic entropy and the maximum of magnetic entropy change is seen at room temperature (≈310K).

k0104

Exploring Magnetic Behavior of Oxalate and Phenanthroline based 1-D Chain Like Molecular Magnet $[\{Cu^{II}(\Delta)Cu^{II}(\Lambda)\}(ox)_2(phen)_2]_n$

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The oxalate (ox) and phenanthroline (phen) ligands based single chain molecular magnet $[\{Cu^{II}(\Delta)Cu^{II}(\Lambda)\}(ox)_2(phen)_2]$ is hydrothermally synthesized. The magnetic properties of the compound are investigated using *dc* magnetization measurements. The room temperature x-ray diffraction measurement s a single phase formation of the compound with space group of $P2_1$. The compound exhibit 1-D chain like structure containing two different crystallographic sites of Cu metal ions (Δ– and Λ–). The Cu transition metal is bridged to oxalate ligands and phen ligand produce π–π interactions within the chain. The *dc* magnetization measurement shows transition temperature of ~75K along with ferromagnetic nature of the compound. The compound exhibit short range magnetic ordering as well over the temperature range ~20-60K.

k0105

Excess velocity of domain walls in amorphous CoFeB thin films

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Domain wall (DW) dynamics have been immensely studied for the last few decades due to rich fundamental physics and spintronics applications. Controlled DW motion has been proposed to use in DW-based race track memory, spintronic memristors, logic units, etc. In particular, DW dynamics plays a pivotal role to understand the DW reversal. Further, disorder associate with DW elasticity leads to various nontrivial effects and DW phase transformation by varying driving field and temperature. There are mainly three different regions (creep, depinning and flow regime) which have been observed in DW motion. Sometimes near the depinning field, the DW dynamics do not follow the universal creep law. The DW velocity (near H_d) is found to be higher than the expected creep law. Previously, this kind of behaviour in DW dynamics has been observed in crystalline ferromagnetic thin films. Here, we have studied the DW dynamics in Pt/CoFeB/MgO multilayer thin films. We have observed the excess velocity in amorphous CoFeB thin films which is well described by the modified creep law. The depinning field (H_d) is found to be ~15mT.

k0106

Tailoring Domain Wall And Relaxation Dynamics In Pd/Co/C_{60}/Pd

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Spin dependent hybridization at the ferromagnet (FM)\organic semiconductor (OSC) interface is very promising for fabricating highly efficient spintronic device. However, the ability of such spin polarized interface on tailoring domain wall, relaxation dynamics and interfacial DM interaction is not understood well. In this context, we have studied the effect of inserting a low spin orbit coupling organic molecule (C_{60}) on the magnetic properties of PMA Pd/Co/Pd sample. The coercivity of the samples reduced systematically by increasing the thickness of the molecular layer. But a striking reduction of bubble domain size is found for a 0.5 nm thin layer of C_{60}. Magnetization relaxation mechanism became much faster in the Pd/Co/C_{60}/Pd samples due to the enhanced domain wall (DW) velocity measured by applying pulsed magnetic field. It reflects that the formation of a spin polarized interface (at Co/C_{60} interface), has reduced the magnetic anisotropy of the sample and enhanced the DW velocity in the creep region. The interfacial DM constant has been deduced for all the samples by asymmetric DW expansion method. Insertion of the molecular layer leads to an increase DMI constant and hence a reduced DW formation energy, which helps in faster DW motion.

k0107

Enhanced Electromagnetic Interference Shielding in Magnetodielectric Layers: A Simulation Study

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In this work, layered structures were simulated and the influence of electromagnetic parameters on the EMI shielding performance of the same was investigated. Simulation results revealed the superior shielding performance of layered structures over individual dielectric and magnetic systems. Further studies on the influence of electromagnetic properties, particularly electromagnetic losses, on the shielding of layered structures demonstrated the importance of incorporation of magnetic materials with high losses in the layered configuration. This study sheds light on the innovation of design strategy of stacked structures designated for suppressed electromagnetic reflections and enhanced microwave absorption

l: ENERGY MATERIALS

l0002

Role of the Sintering Temperature on the Crystal Structural and Oxygen-Ion Conduction Properties of Y2.7La0.3Fe5O12

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The roles of the sintering temperature on the crystal structural and oxygen ion conduction properties of $Y_{2.7}La_{0.3}Fe_5O_{12}$ have been reported. The x-ray diffraction studies confirm that the crystal structure of all the samples sintered between 1200 and 1500 °C are cubic (space group *Ia3d*), however, with an increase in the values of the lattice constant and crystallite size with the increasing sintering temperature. The complex impedance spectra, measured over the temperature and frequency ranges of 40 - 540 °C and 1 – 10^7 Hz, respectively, reveal a thermally activated ionic conduction. The Arrhenius plots relating oxygen ion conductivity show a slope change near the magnetic ordering temperature T_c due to the magneto-electric coupling. With the increase in sintering temperature, the oxygen ionic conductivity increases and the activation energies decreases. Here, we have found a high ionic conductivity (~10^{-2} S/m) at low temperatures (T < 500°C) for the samples sintered at 1500°C.

l0004

Probing Structural Changes in TiO_2 Thin Film Anodes of Li ion Batteries During Discharge

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Coin cell type Li ion batteries have been prepared with rutile TiO_2 thin film electrodes deposited by RF magnetron sputtering on polished stainless-steel substrates. The cell shows a significantly high specific capacity of around 1200 $\mu Ahcm^{-2}\mu m^{-1}$ even after 1000 charging/discharging cycles. Investigations have been carried out on the structural changes of TiO_2 electrodes during discharge of the batteries by synchrotron radiation based grazing incidence X-ray diffraction (GIXRD) and X-ray absorption spectroscopy (XAS) measurements and it has been observed that during discharge of the Li ion battery oxidation state of Ti changes from Ti^{4+} to Ti^{3+} and the lattice also undergoes a structural change from rutile to monoclinic phase. Such information on structural changes in electrode materials during the charging/discharging cycles of a Li ion battery is very important in understanding the long term cyclic stability of its performance.

l0005

Studies On The Screen Printed CdTe Thin Films For Photovoltaic Applications

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We report the synthesis of CdTe powder by colloidal method and then thin films using screen printing technique. The annealed powder in Ar ambient was used to prepare the annealed samples. The optical and structural properties were studied using UV-Vis spectroscopy, X-ray diffraction and Raman spectroscopy. XRD results reveal the growth of cubic

polycrystalline structure of CdTe. TeO2 phase appeared in as-prepared sample was found reduced upon annealing the sample. These results are consistent with Raman results. The intense 1LO peak reveals improved crystallinity of annealed CdTe sample. The decrease in band gap, 1.49 eV (close to bulk value, 1.45 eV) is proposed to be associated to the enhancement in particle size with uniform grain growth.

l0006

Investigation on the Effect of Substrate Temperature of CZTS Layers Grown by RF Sputtering

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We report the growth CZTS (Cu_2ZnSnS_4) thin films using RF magnetron sputtering technique in Argon ambient and effect of substrate temperature. Polycrystalline samples with (112), (220) and (312) reflections were deposited at 300℃ and 400℃ . Thin films deposited at deposition temperature lower than 300℃ shows amorphous nature. (112), (220) and (312) reflections were noticed at about 28°, 47° and 56° respectively. Microstrain shows decrement upon increasing deposition temperature. Crystallite size witnessed rise upon increasing disposition temperature. Dislocation density shows reduction upon increasing deposition temperature. Optical features were probed using UV-Vis technique. Tauc plots reveal the inverse relation of band gap with deposition temperature. Absorbance, transmittance and refractive index values were obtained using UV-Vis technique.

l0007

Benefiting From Less Crystallinity: SnO_2 Anode

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Tin oxide (SnO_2) is an efficient candidate in metal oxide class of anode materials for Li ion batteries (LIB). Although SnO_2 is able to possess high theoretical capacity (1494 $mAhg^{-1}$), the general volume disintegration is detrimental when employed as active participant in LIB. In the present attempt, a less crystalline SnO_2 is prepared along with highly crystalline SnO_2 and a composite of these two was prepared. The prepared composite is checked for anodic properties and compared with regular SnO_2 material. From cycling tests, composite SnO_2 is able to deliver 220 $mAhg^{-1}$ whereas simple SnO_2 delivers 155 $mAgh^{-1}$ for 500 cycles. Also, capacity fading is very low in this composite compared to the unaltered SnO_2 sample, revealing the hopeful choice of this modified SnO_2 as anodic component in LIBs.

l0008

Reduced graphene oxide (rGO)/nickel sulfide nanohybrid as counter electrode in Dye Sensitized Solar Cells

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In the present work, optimally decorated Ni_9S_8 nanoparticles on reduced graphene oxide (rGO) based nanohybrids were synthesized using hydrothermal method for their potential application as counter electrode (CE) in cost-effective dye-sensitized solar cells (DSSCs). The photovoltaic (PV) performance nanohybrid with 40 wt% of Ni9S8 based CE is found to

be comparable to Pt based DSSC and is attributed to their better electrocatalytic activity provided by the synergistic effects of highly conducting rGO sheets and large number of active sites of Ni9S8 for efficient oxidation and reduction reactions

l0009

The Title Goes Here With Each Initial Letter Capitalized Raman Scattering Analysis on Low Energy Kr^+ Ion Irradiated $Y_2Ti_2O_7$ and Y_2TiO_5

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Oxide dispersion strengthened (ODS) steels is considered as the most promising structural material for advanced nuclear systems. The predominant compositions of the dispersoids in the ODS steels are $Y_2Ti_2O_7$ and Y_2TiO_5. In the present work, pellets of $Y_2Ti_2O_7$ and Y_2TiO_5 were irradiated with 70 keV Kr^+ ions at room temperature. Irradiation induced disorder was analyzed in these systems with the help of Raman scattering and transmission electron microscopy (TEM). In the case of $Y_2Ti_2O_7$, there is no significant change in Raman scattering, except for a small change in few peaks. In the case of Y_2TiO_5, majority of the Raman modes (associated with both Y- and Ti- bonds) have broadened upon ion irradiation. The Raman scattering results are in agreement with TEM observations, where krypton bubbles are observed in Y_2TiO_5 but not in $Y_2Ti_2O_7$. It is suggested that more of $Y_2Ti_2O_7$ oxide nanoparticles in ODS steel may improve the high temperature radiation resistance of ODS steel.

l0010

Shape-Controlled SnS Nanostructures: A Wet-Chemical Approach

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Present study reports the successful synthesis of highly crystalline SnS nanoparticles of various shapes/sizes via modified polyol approach. The effect of synthesis parameter (such as refluxing time, solvent, surfactant etc.) on the structural and surface properties of the particles has been comprehensively studied. The study showed that the presence of surfactant and seed based synthesis favors the growth of sheet-like or related morphologies. However, only simple refluxing based synthesis resulted in the development of rod-like feature. Study showed that with the meticulous selection of synthesis conditions with slight modifications, one can result with desired morphology.

l0011

Orientation induced piezoelectric coefficients (d_{33} and d_{31}) in aligned and random fibers of P(VDF-CTFE)

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In this work, the dipole orientation in aligned and random fibers of P(VDF-CTFE) is investigated to see the effective change in piezoelectric coefficients. The prepared random electrospinning fibers of P(VDF-CTFE) show feeble dichroism ($R \sim 1$) and very low (f_m = 0.03) fraction of dipole orientation, while aligned fibers display varying dichroism (R_{max}

~2.24) with large fraction (f_m = 0.29) of dipoles oriented perpendicular to fiber axis. The oriented and uniform distribution of fibers will further enhance the value of piezoelectric coefficients (i.e., d_{33} and d_{31})

l0012

Pressure Induced Current Enhancement in Cu Salt-PVDF Composite

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Combination of poly(vinyldine fluoride) (PVDF) with hydrated copper (Cu) salt in definite proportion shows a drastic enhancement in current, in presence of pressure. The superiority of the composite is attributed to the induced β and γ-phase in PVDF molecule after Cu-incorporation, which is evident from the Fourier transform infrared spectroscopy-attenuated total reflectance (FTIR-ATR) spectra.

l0013

Two-dimensional β-$PdSe_2$ Monolayer For Photovoltaic Applications: First-principles Study

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By employing first principles theory, we demonstrate that two-dimensional β-$PdSe_2$ monolayers is promising candidates for the construction highly efficiency heterojunction solar cells. β-$PdSe_2$ monolayer exhibits a semiconducting nature with an indirect band gap of 1.16 eV. Subsequently, we show that β-$PdSe_2$ monolayer can be used to form type-II heterostructures with the other TMDs for photovoltaic cells. The PCE of β-$PdSe_2$/WS_2(2L), β-$PdSe_2$/P-$PdSe_2$ and, β-$PdSe_2$/$MoSe_2$ excitonic heterojunction can reach 22.8%, 21.79% and 20.3%, respectively

l0014

***In-situ* structural studies on $LiNi_{0.3}Mn_{0.3}Co_{0.3}O_2$ cathode-based Li ion batteries**

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In-situ structural studies has been carried out with synchrotron radiation on Li ion batteries with $Li[Ni_{0.3}Co_{0.3}Mn_{0.3}]O_2$ cathode materials. While *in-situ* X-ray diffraction measurement indicates structural changes during the charging/discharging cycles, *in-situ* element specific X-ray Absorption Spectroscopy (XAS) measurements reveal site specific information. It has been found the major charge compensation at the metal site during charging or Li ion de-intercalation is achieved by oxidation of Ni^{2+} ions without any change in the oxidation state of Co or Mn ions. It is also found that coordination numbers and bond length of Ni-O coordination shells respectively increase and decrease during charging and reverse happens

during discharging, while local structure around Co or Mn sites show much less variation in these parameters

l0015

Spray Pyrolysis Synthesized Zinc ferrite thin film as an electrode for the supercapacitor application.

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Zinc ferrite thin films were deposited on nickel foam by using simple and inexpensive spray pyrolysis technique for electrochemical supercapacitor application. The structural, morphological, and optical properties of synthesized zinc ferrite film were investigated by X-ray diffraction, UV-visible, and FT-IR spectroscopy. The electrochemical measurement of the as-prepared film was carried out by using cyclic voltammetry and galvanostatic charge-discharge techniques.

l0016

Electroactive δ-phase of PVDF Based Piezoelectric Mechanical Energy Harvester

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Piezoelectric electromechanical energy conversion has been studied through poly(vinylidene fluoride) (PVDF) δ-phase film based mechanical energy harvester (MEH). The XRD and ATR-FTIR spectra confirms the formation of electro-active δ-phase in PVDF polymer which is pieo- and ferro-electric in nature. An excellent electrical response is recorded with unpoled MEH (as V*oc* ~ 1 V and I*sc* ~ 600 nA) under gentle finger imparting, but corona poling has shown the significant enhancement in electrical output (as V*oc* ~ 1.5 V and I*sc* ~ 900 nA) in the case of poled MEH comparison to the unpoled MEH. This enhancement leads to the dipole orientation upon the application of electric field.

l0017

Poling Effect on Electrical Properties of KBT based Piezoceramic

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This study explores the structural, dielectric & piezoelectric behavior of $0.97K_{0.5}Bi_{0.5}TiO_3$ - $0.03BiAlO_3$ (KBT-3BA) ceramic fabricated *via* the sol-gel synthesis route. The coexistence of tetragonal (*P*4*mm*) and cubic phase ($Pm\bar{3}m$) was observed in the Rietveld refinement of X-ray diffraction (XRD) patterns of unpoled KBT-3BA sample. The temperature-dependent dielectric analysis of poled KBT-3BA sample showed an additional anomaly which suggests the possibility of electric-field induced structural variation or core-shell microstructure in the system. The ferroelectric to relaxor transition temperature ($T_{F\text{-}R}$ ~ 265 °C) was obtained by the first derivative of dielectric permittivity (ε_r) with respect to temperature (*T*). Further, the

resonance & antiresonance technique was used to determine the depolarization temperature (T_d) ~ 310 °C.

l0018

Synthesis and Transport Properties of P2-type $Na_{0.78}Cu_{0.22}Fe_{0.11}Mn_{0.67}O_2$ Layered Oxide

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Layered oxides are considered the 'holy grail' of cathode materials in ion storage batteries due to their high energy density and easier processing. In this work, a P2-type $Na_{0.78}Cu_{0.22}Fe_{0.11}Mn_{0.67}O_2$ sample was synthesized via a sol-gel method, and its structure and electrical properties were evaluated. Le-Bail fitting of the x-ray diffraction data confirmed the single-phase P2-type structure (space group: $P6_3/mmc$) for the sample. The room temperature bulk conductivity estimated from equivalent circuit modeling of impedance data was ~ 4.5×10^{-4} S/m with an associated activation energy ~ 0.45 eV.

l0019

Density Functional Theory investigation of Mn doped $LiFePO_4$cathodes for Li ion batteries

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Density Functional Theory calculations have been done on Mn doped $LiFePO_4$ system to investigate its structural and electronic properties for differentMn doping concentrations. Effect of Mn doping has been investigated on the lattice constants and unit cell volume of $LiFePO_4$structure.The band gap values have been derived from the density of states calculation which gives an estimation of the electronic conductivity in the Mn doped $LiFePO_4$ system. Li ion diffusion has been simulated using the nudged elastic band (NEB) model and the activation barrier has been compared for the system with different Mn doping concentrations.

l0021

High Performing Triboelectric Nanogenerator Based On Biodegradable Cellulose Acetate Nanofibers

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The accelerated evolution of miniaturized electronics platform has been motivated the development of reliable, wearable and self-powered devices to reduce the dependence on external power source. In this work, the electrospun positive triboelectric layer of cellulose acetate nanofibers with significant triboelectric effect and biodegradable nature has been prepared and integrated with Kapton sheet to fabricate the flexible triboelectric nanogenerator (TENG). Herein, the fabricated TENG demonstrated the conversion of waste mechanical energy ranging from low to high frequency into an electrical energy.

l0022

CdS incorporated polyaniline: High Performance Polymer Based Thermoelectric Composite for Green Energy Harvesting

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Improved thermoelectric (TE) performances with reduced hopping barrier potential have been achieved in hybrid system of CdS incorporated polyaniline (PANI/CdS) composites through an in-situ chemical polymerization technique, for next-generation green energy sources. For exploring the physical properties of the prepared materials XRD patterns and UV-Vis spectra were analyzed. The well-ordered chain packing of PANI and the reduction of carrier hopping barrier with CdS incorporation in the PANI system enhanced the carrier conduction and lead towards better TE properties of this composite. At 100 ^{0}C of the hot end, the highest value of TE power factor (PF) for the composite is found to be 2.61 μW/mK^2. The results indicate that PANI/CdS composite can appear an effective and novel material with improved TE properties of conductive polymers.

l0024

Mechanical Energy Harvesting by Magnesium Salt-Modulated Poly(vinylidene fluoride) Electrospun Nanofibers

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In this work, piezoelectric nanogenerator (PNG) is fabricated by hydrated metal salt ($MgCl_2$•$6H_2O$) (Mg-salt) reinforced polyvinylidene fluoride (PVDF/Mg) nanofibers (NFs) as an active layer and interlocked conducting micro-fiber mats as top and bottom electrodes. The prepared electrospun PVDF/Mg composite NFs having higher content of electroactive phases (i.e., F_{EA}~ 98 %) than that of pure PVDF NFs. As a result, the fabricated PNG generates ~7 V open circuit output voltage under 8 kPa of finger imparting stress.

l0025

Tailoring PEDOT:PSS passivation property by ethylene glycol for PEDOT:PSS/Si solar cells

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Conductive polymer PEDOT:PSS is known as an effective hole transport layer in organic optoelectronics PEDOT:PSS/Si hybrid solar cells (HSCs). It also serves as the surface passivation layer for silicon (Si) thereby reducing the interface recombination losses in the PEDOT:PSS/Si HSCs. However, the mechanism of passivation is not fully established. For better understanding of the role of PEDOT:PSS in Si surface passivation, a systematic investigation of minority carrier lifetime (MCL) for different doping of ethylene glycol (EG)

in PEDOT:PSS is performed on PEDOT:PSS/micro-textured-n-Si/PEDOT:PSS symmetric structure made by spin coating of PEDOT:PSS. The PEDOT:PSS coated Si exhibited an enhanced (~20 folds) value of MCL (~53µs) as compared to that of bare micro-textured Si (~2.5µs) for an optimum EG concentration (7wt%). Further increase in EG concentration has adverse effect on the passivation which is attributed to the segregation of PSS due to excess EG in the matrix. The passivation property of PEDOT:PSS on Si is further demonstrated by detailed quantum efficiency analysis of the Ag/PEDOT:PSS/Si/In:Ga HSCs prepared with different EG concentration.

l0026

Fabrication of efficient PEDOT:PSS/Si hybrid solar cell with 'Back PEDOT:PSS' geometry

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Organic conjugated polymer, PEDOT:PSS and silicon based hybrid solar cells (HSCs) have drawn a significant attention towards efficient and cost effective silicon solar cells. A lot of studies have been dedicated to front PEDOT:PSS device geometry wherein the PEODT:PSS is coated on the Si surface facing the incident light (front side). The PEDOT:PSS acts as an effective hole transport layer as well as passivation layer. However, degradation of PEDOT:PSS caused by environment and the radiation (photo-induced) in such device geometry is a major concern. Here, the hybrid solar cell with inverted structure, Ag/(n-Si/PEDOT:PSS/Ag is fabricated in which PEDOT:PSS is coated on the rear side of the micro-textured Si surface. Maximum power conversion efficiency (PCE) of ~ 2.18% with open circuit voltage (V_{oc}) of 384 mV and short circuit current density of 13.08 mA/cm^2 is achieved. The results are preliminary yet encouraging and require extensive optimization of the parameters. Nevertheless, the 'Back PEDOT:PSS' concept has potential for high PCE and better stability as it provide easy processing with additional advantage of reduced parasitic losses of 'Front PEDOT:PSS' geometry.

l0027

Tea leaf derive carbon dots for high performance Supercapacitor Debabrata Mandal[1], Lalit Bharti[2], and Amreesh Chandra[3]

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Carbon dots quantum dots (CQDs) are fast emerging as next generation nanomaterial for applications ranging from optoelectronic, biomedical to energy field. We present a novel synthesis protocol, to prepare carbon dots quantum dots (CQDs). The prepared CQDs have dimensions in the range of 10-20 nm, as confirmed by TEM and AFM analysis. The graphitic phase formation was confirmed by XRD and Raman analysis. The results clearly show that the materials can be used as electrode materials in energy devices. The electrochemical performance of CQD, in combination with 3M KOH, show that the supercapacitors with specific capacitance as high as ~ 82 F/g and low equivalent series resistance can be obtained. The fabricated symmetric device exhibited a maximum specific capacitance of 44 F/g at 1 A/g current density, with an excellent energy density of ~ 11.2 Wh/kg, along with a power density of ~ 0.5 kW/kg at 1 A/g current density. The symmetric device continues to deliver high coulumbic efficiency and excellent capacitance retention even after 3000 cycles. The

results establish a new protocol for the carbon based material synthesis of CQDs from waste tea leaf.

l0028

Frequency dependence of dielectric properties of modified BCZT lead-free ceramic

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In this research work, $Ba_{0.965}Bi_{0.01}Ca_{0.02}Zr_{0.02}Ti_{0.976}Cu_{0.008}O_3$ (BCZTCuBi) lead-free ceramic has been manufactured by the solid-state reaction method, and its structural and dielectric properties were observed. SEM technique has been used to characterize the microstructural properties of the ceramic and observe a dense microstructure with non-uniform grain size distribution. Further, to understand the role of frequency and polarization contributions to dielectric properties, frequency dependent dielectric analysis of the ceramic sample has been done. Dielectric properties have been studied at different frequencies within the 18 °C to 190 °C temperature range and observed that dielectric permittivity (ε) decreases with the increase in frequency while Curie temperature remains unchanged

l0029

A Facile Hydrothermal Route For Synthesizing β-NiS And Its Electrochemical Performance

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In this work, the ß-NiS nanoparticles are synthesized by a hydrothermal process. The structural study of the sample is analyzed by X-ray diffraction (XRD). Apart from that, in order to investigate the electrochemical performance of the as-prepared material, we carried out electrochemical studies, that is, cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS). The XRD of the sample confirmed the formation of ß-NiS. The study of CV revealed the presence of redox peaks suggesting the faradic reaction taking place at the interface of electrode/electrolyte. The GCD analysis shows that the as-prepared electrode has high specific capacity (194 Cg^{-1} at 1 Ag^{-1}) in 1 M KOH as electrolyte. Further, the EIS analysis suggested the material has good conductivity. The better electrochemical performance of ß-NiS electrode is a future aid to energy field.

l0030

Li Based Quaternarty Heusler Compound LiTiCoSn: A Search of New Thermoelectric Material by First Principle Studies

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In the present research work we explore the structural, electronic, vibrational and the thermoelectric properties of a new Li based quaternary Heusler compound LiTiCoSn, which is recently proposed by Jiangang He et.l. [Chem. Mater. 30 (2018) 4978] that is obeying the 18-electron rule (VEC). Here the theoretical research work is performed within the approach of density functional theory (DFT) and the semi classical Boltzmann transport equations at the constant relaxation time approximation. The calculation of band structure predicts that the compound is n-type semiconductor in nature with the indirect band gap of 0.85 eV. The thermoelectric properties such as Seebeck Coefficient, Electrical Conductivity and Electronic Thermal Conductivity are calculated as a function of chemical potential at the three different temperatures. The compound is found dynamically stable with the cubic (FCC) crystal structure. The maximum figure of merit (ZT) recorded is 0.16 at 700 K temperature. As the compound is first time reporting here; hence the investigations can be the fertile ground to study the material experimentally as well as the practical era of energy conversion techniques.

l0031

Temperature dependence of Raman spectra of Halide perovskites: $Cs_2AgBiCl_6$ and $Cs_2AgInCl_6$

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Halide double perovskite has been attracting attention from the researchers due to its stability and fascinating properties. The potential application of these materials largely depends on temperature of the system, studies related to this aspect are few in number. Using the temperature dependent Raman spectroscopy measurements, we study the phonon decay process of two presently popular halide double perovskites, $Cs_2AgBiCl_6$ and $Cs_2AgInCl_6$, and the preliminary results are presented here.

l0034

Triboelectric Nanogenerator Based On ZnO Nanosheet Networks For Mechanical Energy Harvesting

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In this report, we presented a simple and cost-effective method to fabricate triboelectric nanogenerator (TENG) using ZnO nanosheets. The ZnO nanosheets are grown on aluminium substrate using hot plate assisted hydrothermal method. The ZnO nanosheets film and ITO surface act as triboelectric layers in the TENG. The open-circuit output voltage of ~ 2 V and power density ~ 0.48 μW/cm^2 are generated from TENG in vertical contact separation mode. Subsequently, TENG has the ability to power one Light Emitting Diode (LED) without utilization of any storage element. Therefore, the proposed TENG has potential uses in self-powered sensors and electronic devices

l0035

3D Printed Single Electrode Based Triboelectric Nanogenerator (S-TENG)

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In this work, a S-TENG is developed using micro-patterned 3D printed poly lactic acid (PLA) film as active material with copper (Cu) as single electrode-layer. Triboelectricity depends on contact-separation induced surface charge density between active material and electrode layer that can be manipulated by altering surface chemistry of active material to enhance the performance of S-TENG. Here, 3D printed PLA film is assisted with corona poling is employed to improve surface potential, thus the fabricated S-TENG generates 2 V output voltage under gentle human finger imparting. It is also capable to charge up 1.5 μF capacitor up to 1 V instantaneously. More importantly, S-TENG is possibly utilized as a self-powered pressure sensor which is expected to be a potential candidate for real time motion monitoring, static and dynamic pressure distribution tracing, healthcare and giant monitoring.

l0036

Nickel Ferrite Thin Films for Supercapacitor Application

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The nickel ferrite ($NiFe_2O_4$) thin films were synthesized by chemical bath deposition (CBD) method by using nickel chloride and iron chloride as precursors of nickel and iron respectively and nickel foam as a substrate. The as synthesized thin films were characterized by X-ray diffraction (XRD), Scanning Electron Microscopy (SEM) for structural and morphological studies. The films were further tested for their electrochemical performance. As synthesized Nickel ferrite exhibits the highest specific capacitance of 1976.78 F/g and 302.67 F/g at scan rate 10 mV/s and 100 mV/s respectively. Scan rate increases specific capacitance decreases.

l0037

Ti_3C_2 based two dimensional materials for electrocatalytic activity towards methanol oxidation

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Owing to high cost and poisonous intermediate species of platinum, developing an electrocatalyst with high activity and stability is the main concern for methanol oxidation reaction (MOR). Herein, Ti_3C_2 based two dimensional MXene has been synthesized and explored in MOR. The synthesized MXene is characterized by XRD and SEM. The electrocatalytic behaviour of samples and bare Pt has been studied using cyclic voltammogram curves. The optimized MXene sample shows higher current density (7.726 mA/cm^2) and low onset potential (-0.48 V) which is almost comparable to Pt (8.186 mA/cm^2, -0.50 V).

l0039

Enhanced Dielectric Diffusion With Fe Doping in $Eu_2Ti_2O_7$

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The structural and dielectric property of the pyrochlores $Eu_{2-x}Fe_xTi_2O_7$ have been reported. The structural analysis shows that the $Eu_{2-x}Fe_xTi_2O_7$ has pure pyrochlore phase up to x = 0.2. The dielectric permittivity shows a diffused dielectric transition in Eu2-xFexTi2O7. The increase in dielectric transition temperature and diffuseness with Fe doping have been observed.

l0042

Effect of Temperature on Electrochemical Performance of Activated Carbon FeOOH Composite Electrode for Energy Storage Device

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Low cost, environment-friendly activated carbon-iron hydroxide is synthesized via a low-temperature hydrothermal technique. The structural confirmation is done by verifying its pattern consistency with the JCPDS file. The nano rod-like morphology is revealed by the FESEM technique. The temperature variation, it confirms that temperate rise hinders the contribution of electrolyte ions, so most of them cannot operate at high temperatures may be due to the flammability or volatility of currently used aqueous electrolyte. Which results in increase in bulk resistance of the material in EIS, and decay in specific capacitance value calculated by the CV and GCD. The overall performance of the device is best at the temperature 40^o C.

l0043

Effect of pH on Electrochemical Performance of Molybdenum Selenide: Ultracapacitor Application

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The pH effect on the chemical bonding and electrochemical performance of molybdenum selenide (MoSe2) has been reported in this paper. The samples were prepared via the hydrothermal method and further characterized via Fourier transform infrared spectroscopy (FTIR) and electrochemical workstation (CHI 760). The FTIR confirms the chemical bonds in the prepared samples. The electrochemical performance of the MoSe2 decreases with an increase in pH value from 9 to 11. The M 9 sample exhibits a maximum specific capacitance (Cs) of 156 F g-1 at current density 2 A g-1. It shows an energy density (Ed) of 22 Wh kg-1 at a power density (Pd) of 1015 W kg-1. Hence pH 9 is an optimized condition for high electrochemical performance for MoSe2 nanomaterial for supercapacitor application.

l0044

Structural and Supercapacitor Properties of Chemical Bath Deposited Cobalt Doped Nickel Hydroxide Thin Films

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In present investigation, Cobalt doped nickel hydroxide thin films were deposited on cost-effective stainless-steel substrate by simple chemical bath deposition method. The FT-IR study confirmed the presence of Ni-OH and Co-OH bonds. The electrochemical supercapacitor properties of as synthesized thin films were studied by cyclic voltammetry (CV) and galvanostatic charge discharge (GCD) study. The overall supercapacitor study indicated that 0.6% cobalt doped nickel hydroxide electrode exhibited a maximum specific capacitance of 930 F g^{-1} at a current density of 0.5 mA cm^{-2} in 1 M KOH electrolyte.

l0045

Effect of Molar Concentration of FeOOH on Electrochemical Properties of TiO_2/FeOOH Composite for Supercapacitor

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Transition metal oxides and hydroxides (TMOs and TMHs) have gained wide attention as pseudocapacitive materials for supercapacitors owing to their low cost, high theoretical capacitance, variable oxidation states, and vast abundance. Herein, we report the synthesis of TiO_2/FeOOH composite through a facile hydrothermal route and studied the electrochemical properties of the composite for supercapacitor application. The effect of FeOOH concentration on the performance of the composite was observed. With increasing concentration of Fe^{3+} ions, the specific capacitance of the composite decreased. The composite exhibited maximum specific capacitance of 29.28 Fg^{-1} at 10 mVs^{-1} and specific energy of 0.5 Wh kg^{-1} at a specific power of 175 W kg^{-1} in a two electrode system.

l0046

Enhanced Power Factor Of $Si_{98}B_2$ Added Higher Manganese Silicide Synthesized By Spark Plasma Sintering

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Higher manganese silicides are being explored as the best suitable intermediate-temperature p-type thermoelectric material for waste-heat recovery. Although higher manganese silicides possess low cost, non-toxic and thermally stable constituent elements, their low thermoelectric performance restricts its application compared to other materials in the mid-temperature range. We report an enhanced power factor of higher manganese silicide synthesized using a nano-inclusion approach employing the combination of arc melting and spark plasma sintering technique. An improved power factor ~ 1.40×10^{-3} $Wm^{-1}K^{-2}$ at 773 K was achieved by $Si_{98}B_2$ nano-inclusion in higher manganese silicide material. This power factor enhancement is due to improvement in the Seebeck coefficient, which is imparted from the nano-inclusion composite structuring.

l0047

Cavity and Diffusion Channel Structured $MnMo_6S_8$ Nanoflakes for Flexible Supercapacitor Electrode Application

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In this work, we successfully synthesized $MnMo_6S_8$ nanoflakes by the facile hydrothermal method. Cavities and diffusion channels in its crystalline structure were investigated from XRD patterns. Its nanoflakes-like morphology was scanned by the HR-SEM image. Its functional groups and purity have confirmed from FTIR and EDX spectra. Its electrochemical properties were performed in a three-electrode system. The highest areal capacity of MnMo6S8 modified carbon cloth is 37.7 mC cm^{-2} at a current density of 2.5 mA cm^{-2} was measured from GCD.

l0048

Hydrothermal Synthesis of AgBr as Flexible Electrode Material for Effective Supercapacitor Application

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AgBr nanomaterial was synthesized by hydrothermal method with hexadecyltrimethylammonium bromide as bromide source (CTAB). Morphological and structural studies were investigated using SEM and XRD analysis. Electrochemical performance of the material was examined using three electrode system. The prepared material exhibits the maximum areal capacity of 56.31 mC cm^{-2} at a current density of 1.25 mA cm^{-2}.

l0049

Morphology Tuning of SnO_2 Based Electrode Materials for Supercapacitors

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In this work morphological dependent study of SnO_2 structures for application in supercapacitors is presented. The work revealed that the rutile tetragonal SnO_2 structure can be used as a negative electrode in supercapacitors. The materials were synthesized using two routes viz., co-precipitation, hydrothermal method. The physiochemical characterization was performed using XRD, SEM and BET measurements. The electrochemical characterization of SnO_2 indicates that the performance of particles, synthesized using co-precipitation, is limited due to the low surface area of the particles. Therefore, SnO_2 particles were synthesized hydrothermally, to counter the limiting factors. The stabilized hollow structures lead to appreciable improvement in the performance. The electrochemical properties of all the synthesized materials were investigated by cyclic voltammetry and charge-discharge measurements in 3M KOH, using a three-electrode configuration

l0050

Preparation of Mg ion conducting polymer electrolyte based on PVA and *Nelumbo Nucifera*

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Polymer electrolytes (PEs) based on Poly Vinyl Alcohol (PVA) and Lotus Leaf (*Nelumbo Nucifera* leaf (NNL)) added with Magnesium Chloride ($MgCl_2$) are prepared by simple solution casting technique. The membrane with PVA and NNL gives ionic conductivity in the order of 10^{-6} S/cm for 1gm PVA:300 mg NNL. This composition is optimized one based on ionic conductivity increased from pure PVA conductivity of 10^{-10} S/cm. The sample with 0.2 m.wt% of $MgCl_2$ highest ionic conductivity of $1.805x10^{-3}$ S/cm. Addition of NNL in the PVA matrix enhances its amorphous nature, in which $MgCl_2$ is added as Mg ion donors. A primary Mg ion battery has been constructed with highest conducting sample and open circuit voltage is 1.57V.

l0051

Crystalline Characteristics Dependent Pseudocapacitance Property of $Na_2Ti_3O_7$ as a Negative Electrode for Sodium Ion Supercapacitors

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Layered $Na_2Ti_3O_7$ (NTO) is investigated as a negative electrode for sodium ion supercapacitors owing to its low cost, environmental friendliness, low operating potential and less toxicity nature. Different crystalline features of NTO material were synthesized *via* hydrothermal and facile solid-state route. Solid-state synthesis based NTO material exhibited excellent electrochemical performance with a specific capacitance of 151 F g^{-1} at 1 A g^{-1} current density in 1 M Na_2SO_4 aqueous electrolyte. This enhanced electrochemical performance could be attributed to the higher crystallinity of NTO material. Thus, the material facilitates the intercalation of Na^+ ions during electrochemical processes. Therefore, it is clear that solid-state synthesis based highly crystalline NTO material can be used in high performance sodium ion supercapacitors.

l0052

Effect Of Lithium Doping In Nickel Ferrite Based Hydroelectric Cell

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A hydroelectric cell is an emerging device in the field of green and clean energy generation devices. Defects play an essential role in the adsorption and dissociation of water molecules on the material's surface. We have synthesized nickel ferrite and lithium doped nickel ferrite by ball milling. Lithium doping increases the defects in the nickel ferrite, which improves the output of the hydroelectric cell. X-ray diffraction confirms the cubic spinel structure in both samples. From V-I polarization curves, we observed the maximum output current and output voltage for lithium doped nickel ferrite based hydroelectric cells as follows 40.5 mA and 0.95 volts.

l0053

The Pseduocapacitive behaviour of CeO_2 Nanostructure in Acidic and Organic electrolytes

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The CeO_2 nanoparticles have been synthesized by hydrothermal method. Cerium Nitrate and CTAB was used as the precursor and capping agent respectively. The prepared samples were annealed at 500 ˚C for 4 h. The structural and morphological features of the samples were characterized by XRD, FTIR and SEM. The electrochemical performance of the CeO_2 electrodes has been studied through cyclic voltammetry, charge discharge studies and ac-impedance technique using a three electrode cell. H_2SO_4 and propylene carbonate were employed as electrolytes. The highest specific capacitance of 508 F g^{-1} at a scan rate of 2 mV s^{-1} obtained for 1 M H_2SO_4. Further this electrode exhibits 82.6 % capacitance retention after 2000 continuous charge discharge cycles. All these electrochemical studies reveal that the prepared CeO_2 electrode to be suitable for supercapacitor applications.

l0054

Metal-Organic Framework $[Zn_2(1,4\text{-bdc})_2(dabco)]_n$ as an efficient Electrocatalyst for H_2O_2 Production in Oxygen Reduction Reactions

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Development of non-noble element-based electrocatalyst for oxygen reduction reactions (ORR) through a two-electron pathway to generate hydrogen peroxide (H_2O_2) electrochemically from O_2 reduction. We synthesized $[Zn_2(1,4\text{-bdc})_2(dabco)]_n$ as electrocatalysts, by using 1, 4-benzenedicarboxylic acid (H_2BDC), 1, 4-diazabicyclo[2.2.2]octane (dabco) as an organic linker and $Zn(NO_3)_2.6H_2O$ as metal ion precursor. The structure was characterized and investigated ORR activity by cyclic voltammetry (CV) and rotating ring disk electrode voltammetry (RRDE).

l0055

Optimization of the texturizing process with multi-crystalline silicon wafer for increasing the optical properties

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Multi-crystalline silicon (mc-silicon) ingot was grown using the Directional Solidification (DS) method. The bricks and wafers were sliced from the grown ingot. The aim of this work to analyse the mc-Silicon wafer texturizing for improving the optical properties. Lower reflectance can be obtained by the optimized etching conditions. In this work, we have used the different types of acids in different ratios for texturizing process. Here, we have used HF: H_2O_2: CH_3COOH=3:2:2 (set-1), HF: H_2O_2: $KMnO_4$=3:2:0.2 M (set-2) and HF: H_2O_2:HNO_3:$KMnO_4$ =3:2:2:0.2M (set-3) for etching with the etching time of 60 sec. The HF: H_2O_2:$KMnO_4$ =3:2:0.2M (set-2) gives the better results as obtained from optical microscope and UV- Visible reflectance studies. The etched mc-Silicon wafer surface was analyzed by the optical microscope.

l0056

Structural, morphological, ferroelectric, and dielectric properties of $(0.99)BaTiO_3$-$(0.05)Bi_2O_3$-$(0.05)Nb_2O_5$

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In this study, we have synthesized (0.99)$BaTiO_3$-(0.05)Bi_2O_3-(0.05)Nb_2O_5 -ceramic (lead-free) material via a solid-state reaction method. We have studied the structural, ferroelectric, morphological, and dielectric properties. The formation of a single-phase (tetragonal) perovskite structure with P4mm symmetry was confirmed by powder X-ray diffraction patterns and the average grain size was around the 460 nm range. From P–E loops of the sample, we have found recoverable energy storage density around (W_{rec} ~ 31.32mJ/cm^3) and efficiency (n_{eff} ~ 48.65%).

l0057

Poly(Vinylidene Fluoride-Co-Hexafluoropropylene) Additive in Perovskite for Stable Performance of Carbon-Based Perovskite Solar Cells

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In this study, we improved the hole-transport free carbon-based perovskite solar cells by using polymer additive to passivate the perovskite grains with large size crystals and aid in the growth of polycrystalline perovskite layer with preferred orientation. The fluoro-polymer as an additive into perovskite layer facilitated hydrogen bond with organic cation to form H-F bond, which ought to prevent degradation from moisture. The photo voltaic device with 5 wt% PVDF-HFP additives carried out ~14% enhancement in open-circuit voltage and yielded PCE of 11.1%. It is revealing that the fluoro-polymer enhances passivation of perovskite grains and gives a hope in perovskite photovoltaics.

l0058

Structural and Electrochemical properties of $Sm_{1.5}Sr_{0.5}NiO_{4-\delta}$ Ruddlesden Popper perovskite Material

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In present work, we have studied the Ruddlesen-Popper type of material $Sm_{1.5}Sr_{0.5}NiO_{4\pm\delta}$ prepared by Solid State Route and characterized by XRD and Cyclic Voltammetry. A single-phase solid solution of $Sm_{1.5}Sr_{0.5}NiO_{4\pm\delta}$ having orthorhombic structure with *Fmmm* symmetry is observed. The duck shape of cyclic voltammogram suggests the catalytic regeneration of reactants close to working electrode.

l0059

Enhanced energy storage and dielectric properties of $BaTiO_3$+(0.05 wt.%)Bi_2O_3 and Nb_2O_5 ferroelectric ceramics

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Lead-free ceramics of $BaTiO_3$ + (0.05 Wt. %)Bi_2O_3 – Nb_2O_5 (BTBN) have been synthesized using the conventional solid-state reaction method. The microstructure, electrical properties, and energy-storage performance of the obtained ceramics were examined in detail. The maximum recoverable energy density of 28.21 mJ cm^{-3} with a relatively high efficiency of 46 % was achieved.

l0060

Inelastic neutron scattering studies and simulations on doped $(Bi_xY_{1-x})_2O_3$

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We report inelastic neutron scattering (INS) measurements from 300 K to 1050 K to understand oxygen-diffusion and dynamics in yttria- doped bismuth trioxide. Ab-initio molecular dynamics studies supplement the experimental observations and show that the diffusion of oxygen gets initiated at a lower temperature in comparison to the undoped δ-Bi_2O_3. Although oxygen conduction starts at lower temperature (by about 400 K) at around 700 K, the diffusion is smaller in magnitude. The activation energy required to overcome the energy barrier for diffusion is smaller for the doped systems in comparison to δ- Bi_2O_3

l0062

Fast Cu diffusion in Cu_2Se: An inelastic neutron scattering and simulation investigation

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Here we present the neutron inelastic and ab-initio molecular dynamics investigation on Cu diffusion in Cu_2Se. Our inelastic neutron scattering measurements show strong broadening of phonon spectra in superionic regime that infers the strong anharmonic character of phonon vibrations. The estimated diffusion coefficients (*D*) at elevated temperatures from ab-initio molecular dynamics simulations trajectories lies in the range of superionic conduction. The calculated energy barrier for Cu migration ~0.2 eV, estimated from temperature dependence of *D* is in good agreement with previous reported values. Our simulations show that the Cu hoping in Cu_2Se mostly occurs via octahedral sites.

l0064

Effect of Growth-Temperature on Morphology and Piezoelectric Characteristics of ZnS Nanostructure

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In this work, it has been demonstrated the effect of growth temperatures viz. 140°C and 160°C on the morphology and piezoelectric characteristics of zinc sulfide nanosheets (ZnS-NS) grown on aluminum substrates. An increase in growth temperature has greater influence on the aspect ratio of the ZnS-NS due to the presence of extra thermal energy leading to significant structural deformation which in turn allowed the growth temperature window for the ZnS nanosheets to be determined. The open circuit voltage for the as-fabricated devices

were ~400 mV and ~600 mV, respectively. For the first time, a methodical study was carried out in ZnS-NS system for designing novel piezoelectric nanogenerators.

l0065

Explaining The Improvement In Specific Capacitance Of α-Fe_2O_3 Hollow Sphere Under External Magnetic Field.

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Magnetic supercapacitors have been seen rapid development over the last few years. It has been shown by our team that electrodes having at least one ferromagnetic element can show a significant change in electrochemical performance determined under varying magnetic field environment. This has been mostly attributed to the appearance of Lorentz force and magnetohydrodynamics. Hollow sphere is an effective morphology for supercapacitor electrodes, and the effect of magnetic field on hollow sphere electrode has never been reported. Using α-Fe_2O_3 as a test sample, it is shown that change of supercapacitor performance can also happen, and changes can be quite appreciable. The specific capacitance increases from 73 F g^{-1} to 97 F g^{-1} (at 50 mV s^{-1} scan rate) under the application of a 100 Gauss magnetic field. Also, for 1 A g^{-1} current density, specific capacitance has shown a rise from 73 F g^{-1} to 79 F g^{-1} at 100 Gauss. Modified diffusion behaviour of electrolyte ions near the electrode-electrolyte interface has been considered as one of the main reasons behind performance enhancement.

l0066

The Structural, Dielectric, And Ferroelectric Studies Of Sr Substituted $BaTiO^3$ Ceramics For Energy Storage Applications

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In this study, BTO and 30% Sr substituted BaTiO3 (Ba0.7Sr0.3TiO3) (abbreviated as BTO and BST) have been synthesized via a cost-effective solid-state reaction method. The crystal structure transformed from tetragonal to pseudo-cubic, reducing unit cell volume for Sr substituted BTO ceramic. The Curie temperature (Tc) moved to lower values, from 125ºC down to 40ºC for BST with enhancement in dielectric constant from 4455 to 4785. The energy density for BTO and BST have the same value at 15kV/cm, i.e. 29 mJ/cm^3. However, the enhancement in energy efficiency from 38% to 56.1% can be observed for BST ceramic. The polarization versus electric field loops with low remnant polarization gives minimum hysteresis loss and high energy efficiency for BST compared to BTO ceramic, indicating the suitability for energy storage capacitor usage.

l0067

Cyclic voltammetric study of Organo-metallic electrode sustaining high potential scan rates

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Present work describe the electrochemical performance of the organo-metallic electrodes (OEs) prepared using activated carbon and Ag:$C_{20}H_9ClO_5Ag$ gel obtained from *opuntia cochenillifera* fruit. XRD, FTIR and UV-Vis analyses were used to confirm the formation of material. TEM depicts the formation of spherical and rod like structures with variable sizes ranging from 21.40 nm to 47.21 nm. Cyclic voltammetric analyses in 0.5 M 20 ml H_2SO_4 showed that the electrodes exhibit the structural stability and good performance at scan rate as high as high as $5Vs^{-1}$ within the potential limits – 0.6V and 1.1 V which is higher than any other electrode surviving at that much high scan rate. Prepared electrode exhibits maximum specific capacitance 2.126 F/g at 50 mVs^{-1}.

l0072

Biomaterial Nelumbo Nucifera (Lotus) Leaf - PVA as Solid Electrolyte for Electrochemical Device

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Novel bio-based SPE based on Nelumba Nucifera (Lotus) Leaf–PVA with various compositions of NH_4SCN have been prepared under solution casting technique. XRD analysis has been done to reveal the crystalline/amorphous nature of the membranes. The ionic conductivity has been measured using AC Impedance technique. The conductivity observed for Pure PVA in the order of 10^{-10} S/cm and for the optimized (on the basis of conductivity) 1g PVA+300mg NNL (PN) it is 10^{-6} S/cm. For PN+0.9 M.wt% of NH_4SCN (highest conducting) it is 10^{-3} S/cm, and the OCV obtained by using the corresponding electrolyte for the construction of proton battery is 1.57 V.

l0074

High-Performing Asymmetric Supercapacitor Device Using Nanostructured Co_3O_4 and Fe_2O_3 Based Electrodes.

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The importance of transition metal-based oxides in the field of energy storage is well accepted. Using novel cost-effective synthesis protocols, nanostructured Co_3O_4 and Fe_2O_3 were synthesized. These nanostructures showed impressive electrochemical activity in 1 M KOH electrolyte owing to their redox activity. Further, asymmetric device was fabricated using these two metal oxides as positive and negative electrode, in order to achieve high specific capacitance and excellent energy density. Such supercapacitor devices can be considered as efficient candidate for future energy storage applications.

l0075

Polyvinyl Alcohol (PVA) And Nelumba Nucifera (Lotus leaf powder) based Li-Ion Conducting Electrolytes for Electrochemical Device Applications

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Solid polymer electrolytes (SPE) utilized in the application of electrochemical devices have been prepared based on Polyvinyl alcohol (PVA) and Nelumba Nucifera (Lotus leaf – LL) with the addition of $LiClO_4$ in different weight percentage using solution casting technique. The amorphous/crystalline nature of the prepared electrolytes has been studied using XRD. Ac Impedance analysis is done to identify and measure the ionic conductivity of the membranes where Pure PVA is showing conductivity in the order of 10^{-10} S/cm. In order to increase the ionic conductivity, different compositions of Lotus Leaf powder is added to 1g of PVA and optimized on the basis of ionic conductivity which shows the value of 3.62 x 10^{-6} S/cm for the composition 1g PVA+300 mg LL. And on further addition of salt, the high ionic conductivity is observed as 3.03 x 10^{-3} Scm^{-1} for 1g PVA+300 mg LL+0.7 M.wt% of $LiClO_4$ composition of electrolyte and Li-ion conducting primary battery was fabricated with the highest ion conducting membrane resulting with an OCV of 1.65 V.

l0076

Indoor light harvesting using Bael dye sensitized solar cell

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Dye-sensitized solar cells (DSSCs) are well known as the next-generation solar cells with better solar to power conversion efficiency under low lighting environments (e.g., indirect sunlight). This study aims to determine the performance of Bael leaves extract-based DSSC under indirect sunlight. The photovoltaic properties of the Bael extract sensitized solar cell was evaluated by measuring the open-circuit voltage (V_{OC}), the short-circuit current (I_{SC}), the fill factor (FF), and the maximum power density (P_{MAX}). The parasitic resistance: characteristic (R_{CH}), series (R_S), and shunt (R_{SH}) resistance were measured from the I-V curve. Under a light intensity of (334 Lux), the Bael dye was generated I_{SC} = 0.62 µA and P_{MAX} = 491 nW/m^2.

l0077

Influence of Crucible Dimension In the mc-Si Ingot Growth Process

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We have numerically simulated two 6.90 Kg mc-Si ingot directional solidification (DS) systems (Different ingot dimension: DSS-1 (200 mm * 200 mm * 100 mm) and DSS-2 (158 mm * 158 mm * 158 mm)) by using Finite Volume Method (FVM). The temperature distribution, melt-crystal (m-c) interface shape, vertical temperature gradient and melt flow velocity have been investigated. DSS-1 has convex m-c interface shape and DSS-2 has concave interface shape. Lower vertical temperature gradient and lower melt flow velocity are obtained for DSS-1 compared to DSS-2.

l0079

Influence of Cactus-like Morphology on Supercapacitive Performance of Cr_2O_3

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Cr_2O_3 is considered to be a promising cathodic material for supercapacitor applications on the account of its fast redox kinetics, mesoporous structure, and better electrochemical stability. Herein, we introduced a one-step synthesis of Cr_2O_3 which depicts a unique cactus-like morphology. Such structure improves the specific surface area and ion diffusion mechanism, which enhances the capacitance value. The prepared Cr_2O_3 displayed a specific capacitance value of 35 F g^{-1} at 5 mV s^{-1}, with capacitive retention of ~ 60 % at a scan rate as high as 150 mV s^{-1}. This can be attributed to the redox couple of Cr^{4+}/ Cr^{3+} displayed by Cr_2O_3 at the electrode-electrolyte interface. Hence, cathodic electrodes based on such novel morphology of Cr_2O_3 can be used for devising high-performance supercapacitors, with appreciable chemical stability, and rate performance

l0080

High Performance Na-ion Supercapacitor: Beyond Carbon Structures

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Recent trends in sodium-ion-based energy storage devices have shown a potential use of hollow structures as an electrode material to improve the performance of storage systems. Carbon based material are also the leading material with sodium-based electrode materials. In this paper, V_2O_5 nanorods have been employed as the efficient electrode material for Na-ion batteries. These nanostructures showed impressive electrochemical activity in 2 M NaOH electrolyte owing to their redox activity.

l0081

Role of Minority-spin States and Cu Doping on CO Interaction over Pt_3Cu^- Nanocluster

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First-principles based on dispersion corrected spin-polarized density functional theory (DFT-D3) calculations were performed to investigate the structural properties, relative energetics, and electronic reactivity descriptors (ERDs) of neutral and charged Pt_4, Cu_4, and Pt_3Cu NCs. The interaction mechanism of CO over energetically preferable NCs was examined and our results of ERDs indicate that the doping of Cu atom reduces the strength of CO on Pt atom which can eliminate the poisoning effect of CO.

l0082

Evaluation of Xanthan gum with additive salts as an electrolyte for Sodium-ion Batteries

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The skyrocketing demand of Lithium ion batteries (LIBs) leads to the urge to develop potential energy storage devices. Sodium-ion batteries (SIBs) could be a good alternative due

to its high abundance and cost effectiveness. The replacement of liquid electrolytes with polymer electrolytes is one of the frontiers of enhancing sodium-ion battery competitiveness. An attempt has been made to synthesize a bio polymer electrolyte based on Xanthan gum (XG) with the addition of electrolytic salts such as sodium hydroxide (NaOH) and sodium sulfate (Na_2SO_4) by solution casting method. The complexation between XG and the salt is verified by Fourier transform infrared spectroscopy (FTIR). The ionic conductivity of the prepared electrolytes is measured through AC impedance analysis. The highest conductivity value of $2.9x10^{-5}$ Scm^{-1} is observed for 0.05g Na_2SO_4 incorporated XG membrane which qualifies itself as a prospective electrolyte for sodium-ion battery application

l0083

Enhanced Thermoelectric Properties of Tellurium Excess Silver Telluride Nanoparticles

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Silver telluride (Ag_2Te), a metal chalcogenide, is probable for thermoelectric applications due to its intrinsic low thermal conductivity and high carrier mobility. In the present study, we have synthesized Ag_2Te and tellurium excess silver telluride ($Ag_2Te_{1.1}$) nanoparticles using hydrothermal method. XRD and EDX techniques are used for the phase identification and elemental composition of the samples. Temperature-dependent thermoelectric measurements of the samples were measured in the 313-373 K temperature range. $Ag_2Te_{1.1}$ shows ~ 20 % enhancement in the thermoelectric figure of merit (zT) as compared to the Ag_2Te at 313 K. This enhancement in zT is due to ~ 130 % enhanced Seebeck coefficient and simultaneous ~ 31 % reduction in the thermal conductivity due to the increased phonon scattering at the boundary of the impurity phase present in $Ag_2Te_{1.1}$\

l0084

$ZnIn_2S_4$ Nanostructure For Photoelectrochemical Water Splitting

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In the present work, visible light active zinc indium sulfide ($ZnIn_2S_4$) nanostructure has been synthesized using the hydrothermal method. XRD pattern confirms the formation of a single cubic phase of $ZnIn_2S_4$ (ZIS) nanostructure. SEM and EDS measurements confirm the surface structure and elemental composition of the ZIS sample, respectively. The bandgap (E_g) value of ZIS is observed to be ~2.4 eV using UV-Vis absorbance spectra. The potentiality of ZIS photoelectrode for photoelectrochemical (PEC) activity has been demonstrated. The current density of ZIS photoelectrode under dark and light illumination conditions is observed to be 6.67 $\mu A/cm^2$ and 18.55 $\mu A/cm^2$ at 1 V vs. Ag/AgCl, respectively.

l0086

Defect analysis of In_2S_3 deposited by thermal evaporation by mean of high vacuum treatment

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Di-indium tri-sulphide (In_2S_3), an n-type semiconductor with a variable bandgap, has recently received considerable interest in the solar sector. Thermal evaporation was used to evaporate In_2S_3 powder in this investigation. The structural characteristics of the film were

studied using XRD Photoluminescence spectroscopy was used to investigate the interband defects caused by empty sites in the crystal structure. Instead, surface adsorbed groups appeared on the surface, resulting in the sample being subjected to a high vacuum treatment. This work demonstrates detection of such adsorbed groups by mean of high vacuum treatment.

l0088

A Simple Sonochemical Method of Synthesis of rGO/Co_3O_4 Composite With Binder Free Electrode For Supercapacitors

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In the present work, we have used Phyllanthus Emblica (amla) as a fuel as well as reducing agent to avoid toxic chemicals. rGO/Co_3O_4 composite was prepared by a simple sonochemical method. The electrodes were prepared by using Whatman filter paper without using any binder. The physico-chemical characterizations were performed by XRD, FT-IR, SEM and Raman spectroscopy. Electrochemical measurements were studied by cyclic voltammetry with two electrode system. The result revealed that the composite material has a very good specific capacitance and excellent cyclic stability.

l0089

A Triboelectric Nanogenerator Based on PDMS and Parafilm For Biomechanical Energy Harvesting

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In this report, a triboelectric nanogenerator is fabricated using parafilm, polydimethylsiloxane (PDMS) films for the first time. The fabricated TENG has been used for low-frequency mechanical energy harvesting to drive wearable and low-power electronic gadgets. The parafilm and PDMS layers act as triboelectric layers, and packaging aluminium foil acts as conducting electrodes. A flexible TENG with a dimension of 5 x 5 cm^2 generated an output voltage ~ 8 V and output power of 20.25 μW at the applied load of 1 MΩ. Further, TENG was explored for switching on several LEDs. The current report presents a simple and cost-effective method for fabricating TENG and can be used for self-powered device applications.

l0091

A Numerical Study for Optimizing Performance of Lead-Free Perovskite Solar Cell

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In past few decades, the research on solar cell materials and devices has acquired significant attention, which has contributed into enhancing the performances on even commercial scales.

Moreover, the optimization of various parameters from the aspect of device fabrication has been an important step in this context, and for this purpose, SCAPS simulation has gained enough popularity in recent years. In this work, device optimization has been attempted for lead-free methylammonium germanium iodide perovskite material with p-Si and TiO_2 as hole and electron transport layers (HTL/ETL), respectively, using SCAPS simulation. Results suggest that p-Si could be used as an affordable HTL with adequate device performance.

I0092

Microwave Heat Treatment to Reduced Graphene Oxide (RGO) for Enhanced Electrochemical Supercapacitive Application

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The state of art in improving the porosity of reduced graphene oxide (RGO) prepared via chemical reduction of GO synthesized from modified Hummers method through microwave heat treatment (MWHT) is presented. The prepared RGO before and after MWHT were tested for electric double layer capacitor EDLC type supercapacitor (SC) in a symmetric parallel plate type cell device design. The electrochemical performance of the prepared cell device has been checked from Cyclic Voltagrams (CV) measurements and cross confirmed through Electrochemical Impedance spectroscopy (EIS) and Galvanostatic Charge-discharge (GCD) measurements. After MWHT, the RGO based cell shows enhanced electrochemical performance depicting the enhanced porosity after treatment which hence plays a major role in achieving enhanced specific capacitance.

I0093

Morphology Driven SnO_2 as Electrode Materials for Applications Ranging from Supercapacitors to Sensors

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Metal-oxide nanoparticles are emerging as promising materials for use in supercapacitors as well as in field of sensors due to their inherent surface properties. It is found that SnO_2 can be excellent electrode material for supercapacitors and sensing because of its suitable physio-chemical properties and possibility to perform good redox reaction. In this paper, we present a novel strategy to tune the morphology of SnO_2 nanoparticles from solid to hollow structures. The electrochemical measurements are done in three-electrode configuration. A high specific capacitance of 109 F g^{-1} was recorded in case of hollow SnO_2 particle and 28 F g^{-1} in the case of solid SnO_2 particle-based electrodes. Along with electrochemical characterization, we also report glucose sensing capability. The CV profiles of the hollow and solid SnO_2, before and after the addition of glucose molecules, were recorded in 1 M PBS solution containing 0.5 mM $[K_4Fe(CN)_6]$.The fabricated glucose sensor is able to deliver high sensitivity and low detection limit. This work can initiate significant activity on various applications of SnO2 using hollow structures, which has remained ignored till now.

l0094

Effect Of Gas Flow Pattern On Impurities Distribution In Multi-Crystalline Silicon Ingot Grown By Directional Solidification Process:Numerical Simulation Approach

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In the present study, numerical simulations were carried out for conventional as well as modified gas flow pattern (Inlet gas tube design) in directional solidification (DS) furnace. The effect of modified gas flow pattern on the carbon and oxygen impurity concentrations was studied in detail. The obtained results were compared with conventional and modified grown mc-Si ingots by numerical modelling understanding the impurities segregation during mc-Si growth process by DS model.

l0097

Enhancement of the charge carrier extraction in carbon based perovskite solar cells using $MAPbI_3$:NiO composites

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A variety of approaches utilizing perovskite composites with organic and inorganic materials have been developed to improve the power conversion efficiency (PCE) of PSCs. In this study, we investigated the performance of carbon-based Perovskite Solar Cells (C-PSC) using perovskite composites with p-type nickel oxide (NiO) semiconductor material of varying weight, and the results were compared with C-PSC made with pristine methylammonium lead iodide ($MAPbI_3$) as a perovskite precursor. The single-step method was used to coat the perovskite layers.

l0100

Synthesis, Characterization And Electrochemical Supercapacitor Study Of Mesoporous Cobalt Oxide

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In the present study, mesoporous cobalt oxide (Co_3O_4) nanostructure was synthesized by hydrothermal method followed by annealing treatment. The formation of Co_3O_4 was confirmed by XRD and FT-IR study. The FE-SEM image shows the mesoporous structure. The prepared Co_3O_4 electrode on carbon cloth as a current collector exhibited maximum specific capacitance of 112 F g^{-1} at a current density of 1 mA cm^{-2}. It shows a maximum energy density of 3.15 Wh kg^{-1} and a maximum power density of 630 W kg^{-1}. The Co_3O_4 electrode exhibited excellent cyclic stability of 88.1% over 2000 CV cycles.

l0101

Supercapacitor Performance of the Nickel Oxide Decorated Vertical Graphene Nanosheets Electrode

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The hybrid structures with the combination of carbon nanostructure (EDLC type) and metal oxides (Pseudo type) are gaining attention, due to their high capacitance and superior cycle life compared to conventional storage devices. In the present study, vertical graphene nanosheets (VGN) are decorated with NiO nano-particles using Pulsed Laser deposition Technique. Herein, we report the enhanced electrochemical capacitance of NiOx/VGN hybrid electrodes. As grown VGN exhibited areal capacitance value 0.14mF/cm^2 and it is increased upto 104 mF/cm^2 with NiOx decoration.

l0102
Low temperature processable carbon electrode perovskite solar cell (CPSC) based on SnO2 ETL
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The emergence of perovskite solar cells (PSCs) brings a new era in solar cell research due to their incredible improvement of power conversion efficiency (PCE) within a short span of time. Although PSC has a higher PCE, commercialization remains a big issue. In order to extend the application of PSCs for flexible devices, here we fabricated PSC with low temperature processable SnO2 based electron transport layer (ETL) with a PCE of 7.9%. Additionally, we fabricated a hydrophobic low temperature processable carbon electrode on top of the PSC to address the perovskite layer's moisture instability.

l0103
$SmFe_{0.9}Ni_{0.1}O_3$-Polyanaline Nanocomposite for Supercapacitor Applications
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$SmFe_{0.9}Ni_{0.1}O_3$-Polyanaline (SFO-PANI) composite are prepared by chemical oxidative polymerization method. This prepared nanocomposite was characterized by X- ray diffraction (XRD), and electrical measurements for structural, and dielectric properties respectively. XRD data analysis confirms the orthorhombic crystal structure with Pbnm space group. The dielectric constant show well dispersion with applied frequency. A simple supercapacitor of this material was designed, and was further studied by charging and discharging using $KMnO_4$ (with 0.1M) as an electrolyte. The preliminary designed capacitor show good charge retention capacity and could be a good candidate for future energy storage applications

l0104
$NiMoO_4$-MoO_3 composite as anode material for Li-ion battery application
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$NiMoO_4$/MoO_3 was synthesized by the sol-gel method. The structural properties were studied using XRD and Raman analysis. The prepared sample was used as an anode material for Li-

ion battery. The cycle stability and charge discharge performance of NMO and mesoporous MoO_3 anode were systematically analyzed. The $NiMoO_4/MoO_3$ anode, exhibited a first discharge capacity of 1031 mAh/g and a reversible capacity of 324 mAh/g after 50 cycles. This material is an encouraging candidate for high performance LIBs anode.

l0105

Effect Of Yttrium Substitution At B-Site In $LiCoO_2$ Cathode

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Among various cathode materials used in Lithium ion batteries (LIB), Lithium Cobalt Oxide, $LiCoO_2$ (LCO) is more conventional but suffers with low capacity. In this research work, an attempt has been made to replace the Co^{3+} by Y^{3+} element which is expected to puff up the volume of the unit cell and electrical conductivity. The samples were prepared by sol-gel method and analyzed for structural, morphological and electrical properties. The mixed phase of $LiYO_2$ (LYO) and single-phase trigonal crystal system of LCO was found by X-ray diffraction (XRD) studies and confirmed with TEM-SAED pattern. AC impedance analysis showed a greater electrical conductivity of LYO sample (10^{-4} Scm^{-1}) when compared to the LCO (10^{-5} Scm^{-1}), suggesting a viable option for cathode material for LIBs.

l0106

Preparation of CdS/TiO_2 Heterojunction on Ti Foil for Photoelectrochemical Solar Cell Application

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The CdS/TiO_2 heterojunction have been successfully prepared via electrochemical anodization and chemical bath deposition method on titanium metal foil (Ti). The prepared heterojunction was characterized using X- ray diffraction (XRD), scanning electron microscopy and diffusion reflectance spectroscopy (DRS) techniques. The XRD patterns clearly show the peaks of CdS, TiO_2 and Ti foil. The SEM images of anodized TiO_2 material show nanotubular morphology while CdS exhibits nanopellets like morphology. The DRS is useful to calculate the band gap of TiO_2 and CdS material. The I-V characteristics of heterojunction under dark and illumination is measured.

l0107

Compatible Iron Disilicides Synthesis Employing Reaction Spark Plasma Sintering

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Green power generation and its realisation employing thermoelectric technology mainly depend on non-toxic, environment-friendly thermoelectric constituent materials. Currently, the main focus of thermoelectric research emphasis on earth crust abundance silicide-based materials. Iron disilicides ($FeSi_2$) are one of the silicide family thermoelectric materials; are suitable for mass production and also stable at mid and high operating temperatures. However, the compatibility issues like both n-type and p-type, impede their device applications. In the present study, we report both n-type and p-type $FeSi_2$ synthesis via

suitable doping, employing the combination of spark plasma sintering and vacuum sealing techniques. The synthesized n-type and p-type $FeSi_2$ materials were characterized using the X-ray diffraction (XRD) technique for their phase purity. The significant power factor enhancement was achieved by aluminium and cobalt doping in $FeSi_2$ material.

l0108

Polymer Based Flexible Piezoelectric Nanogenerator For Energy Harvesting Applications

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Barium calcium zirconate titanate ($Ba_{0.85}Ca_{0.15}Ti_{0.9}Zr_{0.1}O_3$, BCZT) ceramic have been successfully synthesised by sol-gel method. The BCZT powder is calcined at 900 ℃, to obtain the single-phase perovskite structure. The flexible BCZT/ Polyvinylidene fluoride (PVDF) films have been fabricated by solution casting method. The particles are homogenously dispersed in the PVDF matrix. β-phase is confirmed by the X-ray diffraction and Fourier transform infrared (FTIR) spectroscopy studies. The dielectric constant increases with increase in weight percentage (wt%) of BCZT in PVDF. The highest dielectric constant is 91.35 and tan δ is 0.05 at 1 KHz.

l0109

Investigation of Reciprocity Between Photovoltaic Quantum Efficiency & Electroluminescence Emission of $CH_3NH_3PbI_{3-x}Cl_x$ Perovskite Solar Cell

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The detailed balanced theory and optoelectronic reciprocity relations between light absorption and light emission is well studied for state-of-the art commercialized silicon solar cell. In this work, reciprocity principle is verified for solution-processed $CH_3NH_3PbI_{3-x}Cl_x$ based planar perovskite solar cells. For this purpose, we utilized the external quantum efficiency (EQE) and electroluminescence (EL) measurements and found a good agreement between calculated and experimental values of EQE and EL. The findings indicates that mixed halide perovskite material has a very small energetic loss to absorption edge broadening ~ 23 meV.

l0110

Simulation of FTO/TiO_2/$CH_3NH_3PbI_3$/CuSCN/C Solar Cell

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The enhanced optoelectronic properties of organo-halide perovskite solar cells have sparked our interest. The cell structure FTO/TiO_2 / $CH_3NH_3PbI_3$ /CuSCN /C is modelled employing SCAPS-1D numerical simulator. The performance parameters of the suggested structure (PCE=13.85%, FF=60.98%, J sc =27.57 mA/cm 2, V oc =0.82 V) match the experimental results well. The influence of absorber thickness and temperature on cell performance is also investigated.

l0111

Corn Husk Derived Micro Porous Carbon: A Promising Electrode Material for Supercapacitor

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Extensive research has been carried out on porous carbon electrode materials for supercapacitor owing to their excellent microstructural properties. In the present study, a renewable resource, abundantly available corn husk is utilized as a raw material for synthesizing the micro porous carbon (MPC) using carbonization followed by chemical activation method. The resultant porous carbon possesses a high specific surface area of 1458 $m^2 g^{-1}$ with dominant micro porosity. A symmetric supercapacitor is fabricated by employing MPC electrodes and maximum specific capacitance of 95 F/g is achieved at a current density of 1 A/g in 6 M KOH electrolyte. Besides, it illustrates excellent rate capability of 92% at high current density of 10 A/g. Hence, this work highlights that the fissile synthesized MPC is believed to be a promising electrode for supercapacitors.

l0112

The structural, optical and dielectric properties of La, Se co-doped BFO

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Pure and Selenium (Se), Lanthanum (La) co-doped BiFeO3, $Bi_{0.92}La_{.08}Fe_{1-x}Se_xO_3$ (L_8Se_x), (where, x=0.1, 0.25, 0.5, 1) nanocomposites were synthesised using sol-gel technique. The structural properties and optical properties of synthesised samples were analysed. Effect of doping in dielectric characteristics of the synthesised samples were studied. Besides, dielectric loss of the samples were investigated.

l0113

Fabrication Of an Efficient $CsPbIBr_2$ Based Carbon Electrode Perovskite Solar Cell Via Organic Cation Passivation

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Perovskite solar cells (PSCs) have emerged as an efficient and advanced solar cell in the realm of solar cells. In which Organic-inorganic and all inorganic PSCs are comparable to silicon solar cells due to their high efficiency. Wherein, cesium lead halide based inorganic PSCs have gained attention of solar cell researchers due to their superior stability compared to organic-inorganic PSCs. Carbon based electrodes have been widely applied in PSCs, as it offers excellent hydrophobicity for all inorganic PSCs and makes the device more stable without the use of any expensive noble metal electrodes. Herein, we have worked on synthesis of good quality $CsPbIBr_2$ layer and fabrication of an efficient CPSC by doping the perovskite with different ratios of Methyl ammonium (MA). Fabricated devices delivered the highest efficiency of 5.1 % and displayed good moisture and thermal stability.

l0115

The $CsPbI_3$ Mediated Electroactive β-phase in PVDF Composite Film for Piezo-phototronic Applications

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In this work, the nucleation of electroactive β-phase in polyvinylidene fluoride (PVDF) film by incorporation of a very low amount of cesium lead iodide ($CsPbI_3$) perovskite is achieved. $CsPbI_3$ is an emerging material with the typical band gap energy ~1.73 eV. Here $CsPbI_3$ interacts with PVDF interfacially and enables to induce electroactive β-phase in PVDF and it also retains the long term stability. Thus $CsPbI_3$ incorporated PVDF composite film turns to be a self-poled film where traditional stretching and poling can be avoided. In the context of green mechanical energy harvesting application, it is expected to exhibit the piezo-phototronic effect that may widen its optoelectronic applications.

l0116

Moving From Solid to Porous Nanostructures for Enhancing the Magnetic Field Dependent Electrochemical Performance of Mn_3O_4 Nanoparticles

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Transition metal oxides have been used as electrode material because of their high pseudo capacitance, chemical stability, and low resistance. Mn-based oxides have been extensively used as efficient electrode material for supercapacitors. Large number of particle morphologies have been investigated to tailor the electrochemical performance of Mn based oxides. The change in specific capacitance, has been directly attributed to the change in specific area. Recently, Mn-oxides have also shown varying electrochemical performance near changing magnetic field environment. But there are no studies, which deals with the possibility of magnetic field dependent variation in these oxides as function of changing morphologies. This should happen because the surface states are known to vary as we move from one morphology to another. In addition, interaction of surface states with magnetic field decides the response of the particles. We report magnetic field dependent electrochemical performance of solid, hollow and porous Mn_3O_4 nanoparticles. It is noted that the hollow and porous structure exhibits the highest specific capacitance of 87 F g^{-1} and 70 F g^{-1}, respectively when 30 Gauss magnetic field is applied.

l0118

Comparative study on the Hole Selective Nature of MoO_3 and V_2O_5 in Carrier Selective Solar Cells

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TMOs with higher work functions like MoO_3 and V_2O_5 are being used as hole selective layer for c-Si solar cells. The dark diode characteristics and capacitance-voltage characteristics of these transition metal oxides with Si are studied with structures fabricated in a diode configuration and illumination characteristics are studied with the TMOs in a solar cell configuration with n^+ BSF on textured Si wafer. The results of the study are compared with previously reported values in literature. Vanadium pentoxide has exhibited a superior hole-selective nature which is evident from the values of the Built-in Potential (V_{bi}) extracted

from Mott-Schottky plot and Open Circuit Voltage (V_{oc}) extracted from the illuminated current- voltage characteristics.

l0119

Ascendancy of Supercapacitive Demeanour of Nickel Doped Cobalt Oxide Thin Film Electrode

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Cobalt oxide was potentiostatically electrodeposited on stainless steel substrates and 2% Nickel was consolidated in the pure Cobalt oxide in the form of thin, uniform films. Both the deposited films were annealed at 500ºC annealing temperature. The X-ray diffraction analysis showed simple cubic crystal structure and Contact angle measurement showed hydrophilic nature of both Ni-doped Co_3O_4 and pure Co_3O_4. The cyclic voltammetry study showed a heave in Specific capacitance from 284 Fg^{-1} of pure Cobalt oxide film to 727 Fg^{-1} of Ni-doped Co_3O_4 at 5mVs^{-1} scan rate in 1M aqueous Na_2SO_4. The charge-discharge scrutiny exhibited accretion in Specific energy from 4.33 $Whkg^{-1}$ to 10.5 $Whkg^{-1}$, Specific Power from 3 $kWkg^{-1}$ to 13.22 $kWkg^{-1}$ on 2% doping of Nickel in Cobalt oxide. Significant supercapacitive behaviour of Ni-doped Co_3O_4 electrode was remarkably observed.

l0120

Bismuth Telluride based High Performance Thermoelectric Generators

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In Bi-Te based thermoelectric generators (TEG) conversion efficiency (η) has been hindered due to poor performance of n-type thermoelectric material as compared to counter p-type material. In present work, we have synthesized polycrystalline n-type thermoelectric material with composition $Bi_2Te_{2.7}Se_{0.3}Cu_{0.01}S_{0.01}$ using high energy ball-mill. We achieved power factor ($\alpha^2\sigma$) value of 1.4 W/m-K^2 in this material which is 50 % higher than the value obtained in commercial n-type Bi_2Te_3 material. Unicouple TEG developed using synthesized n-type material in combination to commercially available p-type $Bi_{0.5}Sb_{1.5}Te_3$ material, exhibits device resistance of 7.5 mΩ. We achieved open circuit voltage (V_{oc}) of 70 mV and load voltage (V_L) of ~35 mV at matching load. With this maximum power output (P_{out}) of ~160 mW is achieved at temperature gradient ΔT of 238 K

l0121

Crystal Structure and Broadband Dielectric Response of $LiPb_2Mg_2V_3O_{12}$ Ceramics

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A low temperature dielectric ceramics $LiPb_2Mg_2V_3O_{12}$ having garnet structure was prepared through conventional solid state reaction route. Its phase purity, crystal structure and broadband dielectric responses were investigated. Rietveld refinement analysis of the compound confirms cubic structure with space group Ia/3d. The observed Raman vibrational modes and group theoretical calculations also confirm the *Ia/3d* space group. At the optimum sintering temperature of 675°C, $LiPb_2Mg_2V_3O_{12}$ possesses a density of 93% and shows a relative permittivity of 8 and dielectric loss of 0.002 at 1GHz.

l0122

Photocatalytic Degradation of Methyl red using Hydrothermally Prepared Cu_2SnS_3 (CTS) Nanoparticles

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Ternary copper tin sulfide, Cu_2SnS_3 nanoparticles were synthesized by hydrothermal method. The structural, morphological and optical properties were studied by using X-ray diffraction, SEM, UV-visible, and FT-IR spectroscopy. The photocatalytic activity of CTS was investigated by for the degradation of methyl red under the visible light irradiation.

l0123

Mechanochemical synthesis of Pure $CsPbBr_3$ and Na-doped Cesium Lead Bromide ($CsPb_{1-x}Na_xBr_3$, x=0.05,0.1 and 0.15), and their Optoelectronic properties

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In this paper, we have synthesized the $CsPb_{1-x}Na_xBr_3$ (x=0, 0.05, 0.1, and 0.15) by mechano-chemical synthesis method at room temperature. X-ray diffraction studies confirmed the orthorhombic phase formation for all the compositions synthesized. Diffuse reflectance spectra obtained for the powdered samples confirmed the absorbance wavelength of around 560 nm for $CsPbBr_3$ and a slight decrease in absorbance wavelength to 515 nm for 5 mol% Na doped sample. Photoluminescence spectra recorded for all the compositions exhibited strong luminescence around 530 nm which is close to that of absorbance wavelength. Direct observation of compositions illuminated under UV short wavelength radiation gave bright green emission. The Na-doped compositions thus developed in this work are being tested further for their stability to humidity, heat and moisture in comparison to the parent phase.

l0124

Study of Isotope Effect in Ti_2CrV-H/D System

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Ti_2CrV alloy has been prepared using arc melting method. Room temperature deuterium uptake (D/M ~ 9) of this alloy is exceptionally higher compared to other Ti based alloys. The body centered cubic (BCC) phase of the alloy has undergone phase transformation to face centered cubic phase (FCC) upon deuterium absorption. Desorption peak temperature of the

saturated deuteride of this alloy is 374 °C which is nearly same to its hydride desorption peak temperature (377 °C). Further DSC studies reveal normal isotope effect in this alloy system.

M: 1-D AND 2-D MATERIALS

m0001

Realizing Half Metallic Gold Nanorods via Platinum Decoration: A First Principles Study

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We have studied the effect of adding a Pt shell on the electronic structure of a freestanding Au nanorod, using first principles based quantum simulation approach. The nanorods are modeled to have a hexagonal cross-section and the simulations are performed using the density functional theory implemented in the SIESTA code. The formation of Pt shell around Au nanorod results in an increase in both the number of nearest neighbours of an Au atom and the lattice constant. Interestingly, we find that the Pt shelling introduces magnetism and half-metallic character in the otherwise non-magnetic and metallic Au nanorods. Tailoring of the electronic band structure in this way can facilitate the realization of future spintronic devices based on noble metals.

m0002

Spin-Drag Rate in a Quasi-One-Dimensional Electron Gas

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In this paper, we calculate the spin-drag rate in a quasi-one-dimensional electron gas (Q1DEG) employing the random-phase approximation (RPA) over a wide range of temperature T, and some selected values of spin-polarization parameter ζ. We find that spin-drag rate is more for the unpolarized case (ζ=0), and it peaks around T~0.25$T_{F\uparrow}$ for all ζ-values. Further the spin-drag rate increases with decrease in the transverse width of Q1DEG, at fixed ζ and electron number density.

m0003

Finite-T Polaronic Effects on the Plasmon-Phonon Modes in a *GaAs* based Electron Quantum Wire

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In this paper, we study the role of polaronic effects on the plasmon-phonon (*pl-ph*) coupled modes in an *n*-type *GaAs* based quantum wire structure. The effect of temperature T is explored on the *pl-ph* modes using the random-phase approximation (RPA) at fixed wire width and electron number density. We find that *pl-ph* excitation spectrum splits into two branches and each energy branch shows blue shift with rise in T. However, the lower branch of the modes get soften in energy as compared to the true plasmon modes of the wire at non-zero T.

m0004

Effect of Etching Time on Structural and Morphological Properties of MXene

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In the present work, two-dimensional MXenes were synthesized using chemical etching method with varying etching times, i.e., 24, 48, and 72 h. The samples were structurally and morphologically characterized using X-ray diffractometer and field emission scanning electron microscopy. It is observed that 24-h-etched MXene annealed at 150°C exhibited pure structural phase of MXene in comparison to longer etching times-based MXenes. The development of TiO_2 nanocrystals is attributed to TiO_2-coupled MXene formed at longer etching times (48 and 72 h)

m0006

Effect of interaction strength on magnetic properties of transition metal doped hexagonal Aluminum Nitride monolayer

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The electronic and magnetic properties of transition metal viz. Mn and Cr doped hexagonal monolayer of Aluminum Nitride is studied using the Green's function based single impurity Anderson model extended to semiconductors by F.D.M. Haldane. The effect of interaction strength was found to be profound in the case of Cr doped AlN and was seen to exhibit good half metallic properties suitable for spintronic applications. Cr was also found to induce a small moment on the neighboring N atoms.

m0008

Anomalous phonons in vertically and horizontally aligned MoS_2

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Recently, vertically aligned (VA) MoS2 has gained popularity due to a potential candidate in gas sensor device applications to detect hazardous and toxic gases such as NO2 as compared to the horizontally aligned (HA) MoS2. Here, we performed a comparative temperature-dependent Raman study on VA and HA MoS2. We observed an anomalous softening, below ~ 50 K, in both systems attributed to the induced strain due to the thermal expansion coefficient mismatch between substrate and MoS2 in a low-temperature regime. Above 50 K, the softening of mode with an increase in temperature is understood by considering the three- and four-phonon anharmonic model. Intensities of the modes as a function of temperature are observed to be strongly dependent on the Bose-Einstein thermal factor

m0010

Electric Relaxation Effect Along with Electric Modulus Analysis in Various Reduced Graphene Oxide–Poly (vinyl alcohol) Nanocomposite

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In this report, we mainly focused the analysis of electric modulus of the four reduced graphene oxide (rGO)–Poly (vinyl alcohol) (PVA) nanocomposite to study the relaxation time (τ_0) and activation energy (E_A). Maximum peak of the frequency dependence imaginary component of the electric modulus has been changed with the change in temperature (30 to120 °C) and rGO contents (wt 5% , 8%,10%. and 12%) in the nanocomposites. The observation showed that E_A increases whereas τ_0 decreases with the increase of the rGO content from 5 wt% to 12 wt% within the nanocomposites. The E_A value increases form 0.125 eV to .251eV with the increase of the rGO content. The characteristic relaxation time in the nanocomposites varies from a minimum $5.25*10^{-8}$ sec to a maximum $3.25*10^{-7}$ sec.

m0012

Effect of M and S_2 Vacancies at Different Sites on MS_2MLs (M = Mo, W): An *Ab initio* Study

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The effect of vacancies (M (= Mo, W) and S_2) on structural and electronic properties of MS_2MLs (at different vacancy concentrations) have been studied. With the decrease in percentage of vacancy concentrations the magnitude of binding energy increases. These vacancies help to tune the electronic band structure by creating additional acceptor and donor levels near Fermi and hence suggest their applications in electronics.

m0013

Layer dependent anomalous Raman scattering in T_d-WTe_2

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Tungsten ditelluride (WTe_2) is a Weyl semimetal belonging to the class of layered transition metal di-chalcogenides (TMD). It shows exotic properties like high magnetoresistance, large thermo-emf, anomalous Hall effect *etc*. The electronic properties are strongly related to its crystal structure and change drastically on the reduction of thickness of the crystal from bulk to a few layers. Through systematic layer-dependent Raman spectroscopy studies, we show how the point group symmetry of the crystal changes from bulk (C_{2v}) to monolayer (C_{2h}). Redshift and evolution of few characteristic Raman modes (for example, $A_1{}^3$ mode, centered at ~115.7 cm^{-1}) are analyzed to investigate the anomalous behavior.

m0014

Asymmetric Negative Differential Resistance Behavior in Ag/TiO_2/FTO based Resistive Switching Memory Device

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In this work, we performed an investigation on the memristive effects on TiO_2 nanorod arrays (TNAs) based RRAM devices, grown on FTO coated glass substrate via hydrothermal technique. According to our experimental results, the device exhibited a hysteretic current-voltage behavior which shows the memory effect along with the negative differential resistance (NDR) state in both the positive and the negative biases.

m0016

Energy-loss in Graphene superlattice

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An interest has been sparked off in graphene based multilayer (GBM) and graphene based superlattice (GBS) structures because of their potential applications in technology. This paper consists of theoretical investigation about energy-loss of GBS within Random Phase Approximation (RPA). The energy-loss is dependent on the charge density and separation between layers of GBS. As the charge density is increased the intensity of energy-loss is increased. With increase in distance between the layers the zero energy-loss regions is less compared to more compact GBS. Thus GBS can be considered as better device making material with lesser energy-loss than SLG. This low energy-loss in GBS can have better technological applications as energy storage devices.

m0017

Characterizations of a Few Layered MoS_2 Phototransistor Using a Homebuilt Cost Effective Measurement Setup

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Having an atomically thin profile, semiconducting transition metal dichalcognides (TMDC) promising 2D materials for electronic and optoelectronic device applications. In this work, a phototransistor based on the mechanically exfoliated few layered MoS_2 nanosheet is fabricated, and its light-induced electric properties are investigated using a low cost homemade setup. This device shows excellent switching behavior (10^4) and higher photoresponsivity (4.51×10^6 A/W) at a low bias (V_{ds} =1V), making it promising for technological applications.

m0018

Amplification Of Phonons In Undoped Bilayer Graphene In The Presence Of External Temperature Gradient

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We present a theoretical investigation on the amplification of acoustic phonons interacting with electrons confined in Bilayer graphene (BLG) due to external temperature gradient (∇T) by using Boltzmann transport equation approach. From our research work, we investigated that for T=77k, the calculated value for ∇T is found to be $3.2063 \times 10^{-23}\mathrm{K/m}$ whereas for Single layer graphene (SLG) it comes out to be 30.478K/cm as reported in Ref[2].

m0019

Designing an Efficeint Sensor Based on Penta-graphene for Detection of Formaldehyde

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Here we have studied the adsorption of formaldehyde (H_2CO) on penta-graphene (PG) and finds its application as a gas sensor using density functional theory (DFT) calculation. It is found that formaldehyde is physisorbed on penta-graphene with small binding energy and a large binding distance. We find that the major contribution to the adsorption energy comes from the van der Waals London dispersion interaction (LDI). Our calculation suggest that penta-graphene is a promising material for designing gas sensor for detecting formaldehyde.

m0020

Oxidation Study of Titanium Carbide ($Ti_3C_2T_x$) Using A Thermo-gravimetric Analyzer

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MXene is a novel 2D material to be utilized in many applications. Titanium carbide $Ti_3C_2T_x$, because of its versatile properties, is the most extensively researched MXene. Although it is an extremely promising candidate for several applications, such as superconductors, batteries, electromagnetic shielding, and sensors, its storage in the air is a challenge. We have synthesized $Ti_3C_2T_x$ with the HF etching technique to investigate this. XRD measurements ascertain the composition of the synthesized material to be the hexagonal structure of titanium carbide, while the imaging has been done by using FESEM. Here, we propose the study of the oxidation stages of $Ti_3C_2T_x$ in the air which are being examined using a thermo-gravimetric analyzer (TGA).

m0021

Structural Evolution of Molybdenum Phosphate

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Metal Phosphates, particularly the layered metal Phosphides and phosphates, have gained much attention from the research community. Molybdenum phosphate is one of the promising class of transition metal phosphates (TMPOs). In this report we intend to study the synthesis, structural, and morphological variations of molybdenum phosphate nanomaterial. A facile hydrothermal approach is carried out for synthesizing molybdenum phosphate and investigated by X ray diffraction (XRD), Thermogravimetric analysis (TGA), Fourier transform infrared spectroscopy (FTIR), Scanning electron microscope (SEM). The result indicates the formation of $(NH_4)_{2.6}$ $(H_3O)_{0.4}$ $(PMo_{12}O_{40})$ Ammonium Oxonium Dodecamolybdophosphate which was further annealed at 250 ºC, 350 ºC, 450 ºC temperatures to get the pure form.

m0023

Effect of Carbon Cloth Substrate on Field Emission Properties of Bi_2S_3 Nanostructure

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In present study, Bi_2S_3 nanostructures are grown on carbon cloth via facile hydrothermal route in order to investigate their FE properties. The physico-chemical properties of synthesized Bi_2S_3 nanostructures were studied using various characterizations such as X-ray diffraction (XRD), Scanning electron microscopy (SEM) etc. The SEM micrograph illustrates the Bi_2S_3 nanorods are vertically grown on carbon cloth. The FE study reveals, Bi_2S_3 nanorods grown on carbon cloth delivers maximum current density of 2167 $\mu A/cm^2$ at an applied electric field of 3.2 V/μm with lower turn-on (defined at 10 $\mu A/cm^2$) and threshold field (defined at 100 $\mu A/cm^2$) of 1.48 and 1.82 V/μm, respectively than pristine Bi_2S_3 nanostructure. The emission current stability tested at a pre-set value of ~2 and 5 μA over 4 hours duration is observed to be very good. The superior FE characteristics are attributed to the high aspect ratio of the vertically oriented nanorods, their excellent mechanical and chemical sturdiness, and intimate contact with the electrically conducting carbon fibers. The outcome of FE properties indicates the potential applicability of Bi_2S_3 nanostructure emitter grown on carbon cloth in the practical application in FE based vacuum micro/nano-electronic devices.

m0024
Substrate Dependent Growth Study of $ZnIn_2S_4$ Nanostructures Formation by Single Step Hydrothermal Method
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The unique structural features and fascinating physicochemical properties of 2D nanostructured materials have shown great application in charge storage, optoelectronics and photoconduction device. Zinc Indium Sulfide ($ZnIn_2S_4$) is the only member of the ternary metal sulfides family with a layered structure. Amongst the methods used for synthesizing $ZnIn_2S_4$ structures, the hydrothermal technique offers a simple, cost-effective and environmentally friendly route for materials synthesis. To study the effect of substrate on the formation of hydrothermally grown $ZnIn_2S_4$ on several types of substrates were used. The structures of the $ZnIn_2S_4$ were systematically studied by scanning electron microscopy (SEM) and XRD. It was demonstrated that the type of substrates used had a great influence on the morphologies, density and alignment of the $ZnIn_2S_4$ formed. The ordered structure of nanometric dense $ZnIn_2S_4$ has been prepared on the conductive substrate for practical application in nano electronic devices.

m0025
A Comparison of Transient Optical Response of a Monolayer MoS_2 near to its A, B, and C Excitons

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Ultrafast carrier dynamics study has been performed on monolayer MoS_2 at three excitonic transition energies by pumping and probing with corresponding photon energy. Measurements at A and B excitons peaks show an initial negative maximum in ΔT/T which recovers within the first few picoseconds. At a later time, a positive maximum in ΔT/T has been observed only in the case of measurement at A exciton. At C exciton, ΔT/T remains positive throughout the first 15 ps. The recovery of ΔT/T in the case of both A and B excitons are of similar time scales, whereas C takes a much longer time. The origin of such transient changes in transmission has been explained through various ultrafast physical processes in the MoS_2.

m0027

Impressive Electronic and Optical Properties of HfN_2/ $MoSe_2$ Heterostructure: A Density Functional Theory Study

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The electronic and optical properties of bilayer HfN_2/$MoSe_2$ Van der Waals heterostructure have been investigated using density functional theory (DFT). The HfN_2/ $MoSe_2$ heterostructure has been constructed by two types of stacking (AA′ and AB) of single layer $MoSe_2$ and HfN_2. Both the stacking has direct band gap though AB stacking has a slightly higher band gap than AA′ stacking. It is also observed that the AB stacking is more sensitive to the spin orbit coupling (SOC) effect. The HfN_2/ $MoSe_2$ heterostructures have high value of absorption coefficient in the visible and ultraviolet regions. Our theoretical investigation suggests that HfN_2/ $MoSe_2$ heterostructure can be very promising candidate in nano electronics and optoelectronics for visible and ultraviolet photodetector.

m0028

Study of the electrical modulus spectrum to the analysis of electric relaxation and conductivity effect in Graphene Oxide – PAA Composite

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In this report, we mainly focused the analysis of electric modulus and AC conductivity of the two-graphene oxide (GO)–Poly (acrylic acid) (PAA) nanocomposite to study the electrical properties and relaxation effect. Maximum peak of the frequency dependence imaginary component of the electric modulus has been changed with the change in temperature (20 to110 °C) and GO contents (wt 5% and 10%) in the nanocomposites. The observation showed that activation energy (E_A) decreases whereas relaxation time increases with the

increase of the GO content from 5 wt% to 10 wt% within the PAA-GO composites. AC conductivity within both sample increases with the increase of temperature and frequency in the range 10^{-4} to 8×10^{-4} S/m. The E_A value decreasesfrom 0.256 to 0.121eV with the increase of the GO content.

m0029

Stability and Electronic Structure of Novel Allotrope of Two-Dimensional Platinum Disulfide

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The stability and electronic structure calculations of the novel monolayer allotrope of PtS_2 have been performed using density functional theory and the G_0W_0 method. Stability analysis reveals that the monolayer allotrope is free from imaginary modes that suggest its dynamical stability. The electronic structure calculations show an indirect band gap of 1.57 eV and 3.04 eV at the GGA-PBE and G_0W_0 level of theory, respectively. The strong hybridization of Pt-d and S-p states forms the top of the valence band and the bottom of the conduction band. The bands nearest to the Fermi level are independent of SOC effects. However, strong splitting of Pt-d bands below the Fermi level has been observed. These characteristics make monolayer PtS_2 a candidate material for optoelectronic applications.

m0030

Antibacterial Behavior of Salt Assisted Chemically Exfoliated MoS2 Nanosheets Against Pathogenic Strains

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The 2D MoS2 nanosheets have been fabricated by systematic salt assisted exfoliation of bulk powder. The synthesized nanostructures were characterized using x-ray diffraction (XRD), high-resolution transmission electron microscopy (HRTEM) and energy dispersive X-ray spectroscopy (EDS) measurements. The interlayer spacing obtained from HRTEM analysis of exploited nanosheets is in good agreement interlayer planes spacing of the XRD analysis. The antibacterial potential of synthesized 2D nano-structure were evaluated against one gram positive (Bacillus Subtilis) and two gram negative (Escherichia Coli and Pseudomonas Aeruginosa) pathogenic strains. The experimental results clearly showed significant resistance of exfoliated MoS_2 nanosheets against Bacillus Subtilis and, minute effect on Escherichia Coli and Pseudomonas Aeruginosa at low concentrations. The antibacterial behavior is attributed to generation of reactive oxygen species (ROS) on MoS_2 nanosheets surfaces.

m0031

Electrical Properties of Carbon Dots Extracted From Biomass

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We report optoelectronic properties of carbon dots, extracted from microbial biomass as obtained after protein purification under centrifuge method. Electrical properties of synthesized carbon nanodots was examined in thin film form, when sandwiched between transparent conducting substrate and thermally deposited aluminum electrode on it. Optical absorption and photoluminescence studies of carbon nanodots depict semiconducting nature of the materials, which was further confirmed by electrical measurements. Our studies open up a new form of semi-conducting organic nanocarbon materials (after inorganic carbon nanotubes and graphene) for their applications in chemical sensor, bio-imaging, nano-medicine, light-emitting diode (LED) and renewable energy resources.

m0032

Enhanced gas response of mechanically activated WS_2 flakes towards NO_2 gas at room temperature

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Activated WS2 is prepared using ball milling technique and characterized its nature using XRD and Raman spectra. The WS2 samples were coated as sensing films and its chemiresistive properties towards NO2 gas molecules were analyzed. The 1h WS2 sampled showed effective response with enhanced response and recovery time. Due to long time, mechanical disruption of the 2h WS2 sample lead to decreased response rate compared to pure and 1h WS2 samples. Therefore, controlled activation of layered structures enhances its effective properties towards real life application.

m0033

Electronic and Optical Properties of 2D Janus BiTeCl Compound

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Taking inspiration from the successful experimental synthesis of two-dimensional Janus BiTeCl and BiTeBr compounds, we report electronic and optical properties of monolayer BiTeCl using state-of-the-art density functional theory. The spin–orbit couplingeffect show significant reduction of band gap of BiTeCl monolayer. The calculated direct bandgap value of BiTeCl is 0.84eV with GGA-PBE+SOC functional as compared 1.7 eV at GGA-PBE level of theory. The optical absorbance spectra of BiTeCl lie in the UV-visible region having a peak at 2.7 eV. The moderate value of band gap and strong light absorption ability makes BiTeCl monolayer to be potential candidate for future electronic and optical devices.

m0034

Magnetic Properties of Cr_2O_3 Nanosheets

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We present a study of the structural, morphological and magnetic characterization of the magnetoelectric Cr_2O_3 nanosheets, synthesized by a rapid thermal annealing method. The crystal structure of these nanosheets is found to be rhombohedral with space group R-3c. The results of magnetic measurement of these nanosheets reveal antiferromagnetic behavior with the Neel temperature ~285 K. Moreover, the low temperature isothermal magnetization

behavior was shown to exhibit small hysteresis loop and absence of spin flop transition, which is in contrast to the magnetic properties of the bulk and nanoparticle Cr_2O_3 samples.

m0035

Single-electron transistor based on Bi_2Te_3 and Sb_2Te_3 island

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Topological insulators are a new class of material where the bulk is insulating in nature but the time-reversal symmetry-protected surface states are conducting in nature. In this work, we have compared the operation and performance of a single electron transistor based on two topological insulators: Bi_2Te_3 and Sb_2Se_3. From the analysis of the gate voltage-dependent total energy, the electrostatic coupling between the gate electrode(s) and the island (α_{avg}) and the electrostatic polarization parameter (β_{avg}) towards the total energy were calculated to be 0.23667, 0.04 eV^{-1} for Bi_2Te_3-SET and 0.159, 0.03 eV^{-1} for Sb_2Se_3-SET. Also, from the charge stability diagram, we found the first addition/ejection of an electron occurs at a slightly lower voltage for Sb_2Te_3-SET and the separation between the voltage at which the addition/ejection of electron happens is also slightly higher for the same.

m0036

Flicker Noise in an Electrolyte Gated Large Area Gr-FET

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Here, we report low frequency noise measurement in a top gated CVD graphene device using a lock in amplifier-based ac technique at room temperature. We tune the carrier density of graphene by electrolyte-gating through which a wide range of carrier density can be accessed due to formation of nanometer thick Debye layer at the gate interface, offering large capacitance. The power spectral density mostly follows 1/f type behavior. By varying the carrier density, the noise magnitude shows a dip near the charge neutrality point and increases with density. The behavior is unusual compared to the reported data on exfoliated graphene device and can be explained through the charge exchange between the interfacial traps and graphene.

THESIS PAPERS

t0005

Preparation and Characterization of Thin Film Multilayer Devices for Application in Water Window Regime of Soft X-Ray

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The present thesis describes detail experimental investigations carried out on three important thin film multilayer (ML) systems viz., Co/Ti, Cr/Ti and Cr/Sc which theoretically possess high reflectivity in water window regime (2.3-4.4 nm) of soft X-rays. In this thesis work, these ML's have been prepared by magnetron and ion beam sputtering techniques and have been characterised mostly by specular X-ray reflectivity, diffused X-ray scattering and cross-sectional TEM. Since it is well known that interface imperfections i.e., roughness and diffusion at the interfaces and their propagation across a ML is very critical for its performance as a device, the main focus of this work has been to characterise the buried interfaces of the ML's thoroughly using various techniques and to reduce the interface imperfections by application of barrier layers. Among various important results, the high soft x-ray reflectivity valueof 31%at 2.77 nm for Cr/Ti ML with C barrier layer,obtained in course of this thesis work, is most remarkable as it is the highest reflectivity reported so far in the literature in this wavelength regime of water window.

t0006

Chemical Vapor Deposition Grown MoS_2 for Sensing Applications

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During my PhD, I have published 18 peer-reviewed international journals including ACS Sensors (2), Applied Physics Letter (2), Advanced materials interface, Advanced materials technologies, Nanotechnology (4), IEEE Sensors (2) etc. I fabricated a room temperature NO_2 gas sensor using CVD grown 2D MoS_2. That discovery removes the microheater from commercial solid-state gas sensor technology through detecting target gas molecules at room temperature. Moreover, the main issue of 2D materials-based gas sensor is incomplete recovery at room temperature which was rectified by exploiting the synergistic effect of 2D material and metal oxide semiconductor through synthesizing a hybrid of MoS_2 and MoO_3 via nucleation-controlled one-step CVD process. I also fabricated a high-performance photodetector in visible spectra without applying gate voltage by synthesizing a vertical out-of-plane van der Waals heterojunction of MoS_2 and reduced graphene oxide. My research outcomes and interesting results help to synthesis pure low dimensional materials at large scale and address main challenges in chemical and light sensors.

t0009

Formation of Hierarchical Nanostructured Micro-granule by Self-assembly and its characterization by Small-Angle Scattering

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The broad objective of the thesis is to understand certain novel phenomena in the correlated nanostructure of micro-granules. To investigate the structural correlation, hierarchical nanostructured 3D micro-granules have been realized by rapid drying of contact-free

colloidal droplets using spray-drying. The thesis aims to establish a correlation between physicochemical attributes with the formation of the novel granular structures by evaporation induced self-assembly. The thesis is focused primarily on four aspects; i) The effect of nanoscale confinement in the granules, ii) The role of trapped water in nanoscale pores towards novel properties of the granules, iii) The role of competitive interfacial interactions during evaporation induced self-assembly and its influence on resulting structural correlation, and iv) The effect of colloidal shape anisotropy to tune the structural correlation. Moreover, the thesis explores plausible applications of such novel nanostructured micro-granules. Apart from the investigations on the nanostructured micro-granules, the thesis also presents the development and installation of the country's first synchrotron based Small-Angle X-ray Scattering beamline at Indus-2 synchrotron, RRCAT, Indore

t0010

Signatures Of Criticality In Abrupt Metal-Insulator Transitions

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This thesis is dedicated to the observations of criticality in a class of well-studied solid-state materials undergoing thermally-induced first-order phase transitions. Our focus is on the necessarily hysteretic abrupt phase transitions seen in the transition metal oxides such as V2O3 and VO2, magnetocaloric materials and intermetallic alloys, manganites, etc. The phase transition in these materials is unambiguously falls in the category of abrupt transitions because of the observed hysteresis and a large latent heat. Our experimental work shows that such transitions also exhibit features that are considered the hallmarks of the critical (second-order) transitions---dynamic scaling, critical phase-ordering dynamics, and critical slowing down. The origin of these features is attributed to the spinodal singularities. We argue that this mean-field behavior results from the suppression of fluctuations on account of the long-range strain fields resulting from the structural transition that often accompanies the electronic or magnetic transitions.

t0011

Influence of Local Structure on the Magnetism of Mn-Based Novel Heusler Alloys

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This work discusses the varied magnetic states observed in some unconventional Mn-based Heusler alloys. To understand the ground state properties of these materials, a closer look has been taken at their structure with different probes such as synchrotron x-ray, neutron diffraction, and x-ray fine structure studies. We have chosen to synthesize three distinct group of Heusler systems with Mn as their main magnetic contributor, in view of a complex nature of atomic bonding. Firstly, Ga_2MnCo and three analogous compositions belonging to the very new Z_2XY family of Heusler compounds with dominant *p-d* hybridization are studied. Secondly, the $Ni_2MnSb_{0.5}Z_{0.5}$ (Z=Al, Sb) composite Heuslers are investigated for their emerging magnetic properties, and lastly, NiFeMnGa along with two new quaternary Heusler compounds are explored for their potential spin-polarized nature. In all the above systems, we find exceptional magnetic ground states, which further unveils hitherto unidentified abnormalities occurring at local atomic order.

t0013

Physical Properties and Related Phenomena in Some Selected Rare-Earth Transition Metal-Based Perovskite Compounds

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The thesis entitled ''*Physical properties and related phenomena in some selected rare-earth transition metal-based perovskite compounds*" has several important aspects which have been described from the experimental and theoretical prospective. To serve that purpose, several oxide-based perovskite compounds such as doped manganite and double perovskite systems with different magnetic and electronic ground states have been prepared. The structural and physical properties of the as-prepared compounds have been investigated in detail.

t0014

Anomalies in the Dirac states – a high-resolution photoemission spectroscopic study

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Topological materials have drawn much attention due to their importance in quantum applications. While many such materials have been predicted theoretically, experiments show anomalies in the properties of Dirac fermions. We have investigated two such materials; BiPd (a noncentrosymmetric superconductor) and graphene grown on SiC substrate employing high-resolution hard x-ray photoemission spectroscopy (HAXPES) and angle-resolved photoemission spectroscopy (ARPES). In the experiments, we identified surface-bulk differences in the electronic structure of BiPd and the momentum of the Dirac fermions. We showed that Dirac fermions are the surface states and possess unusual anisotropy. We proposed a model Hamiltonian to capture the anisotropic properties of this system. Our results on graphene reveal the typical band dispersion of the Dirac bands across the node which has been debated for long. We also show that the properties of the Dirac states remain unchanged even if the system is perturbed by chemical substitutions thereby changing the density and mobility of the charge carriers. These results provide an understanding of long standing issues, and can have immense implication in quantum applications.

t0015

Biobased Silica from Rice Husk and Straw for the Synthesis of Biocompatible Glasses

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In this modern era, the research on innovative materials and techniques for applications in the medical field improved the quality of life considerably. It reduced the treatment costs of several diseases. Among materials for biomedical applications, bioactive glasses have been widely studied, since the 1970s, as third-generation bone substitutes and biomaterials for tissue regeneration. The term "bioactive" is related to the ability of these glasses to stimulate bone regeneration through a peculiar reactivity that induces the formation of a hydroxyapatite layer on their surface. A typical property of bioactive glasses is the possibility of being doped with ions of therapeutic interest. The present work aims to investigate the preparation of

bioactive glasses by using rice husk derived silica. The glasses have been synthesized by the traditional melt-quench method. The obtained glasses have been subsequently characterized in terms of their characteristic temperatures by Differential Thermal analysis (DTA/DSC), phase analysis by X-ray diffraction (XRD) and structural analysis through spectroscopic techniques (Scanning electron microscopy, energy dispersive X-ray spectroscopy and Fourier-transform infrared spectroscopy - FTIR). In addition, the obtained bioactive glasses were immersed in solutions similar to biological body fluid to investigate their bioactivity, evaluating pH of solution with time, ion release with the help of microwave plasma spectroscopy and hydroxyapatite formation. The findings suggested that incorporating different oxides (MoO_3, SrO, MnO, CoO) into a bioactive glass does not give any negative effect. This provides beneficial role for the synthesis of a new class of bioactive glasses for drug delivery and antibacterial activities. The entire work in the thesis is presented in ten chapters.

t0016

Investigations On Certain Lanthanide Doped Zirconate Perovskites For Optoelectronic Applications

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The study of luminescence properties of rare-earth elements hosted in several crystalline matrices is strongly motivated because of their potential applications in optoelectronic devices and flat panel displays. This thesis investigates the possibility of tuning the luminescence properties of different rare earth doped single phase perovskites systems for producing white light emission. It is observed that different systems synthesized during this entire research work yield emissions that cover different regions of the visible spectrum; that too with appreciable intensity. Pleasant warm white light is achieved for $CaZr_{0.90}Sm_{0.025}Dy_{0.075}O_3$ system excited at 354 nm with CIE coordinates (0.3310, 0.3349). Results indicate that both powder as well as film samples prepared during this work can find applications in various display and optoelectronic devices based on their emissions in different parts of the electromagnetic spectrum.

t0017

Understanding Magnetocaloric Properties Of Mn Based Antiperovskite Materials

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The thesis aims at understanding the effect of substitution and vacancy on the magnetostructural and magnetocaloric properties of Mn_3SnC antiperovskite compounds by introducing changes at all three sites. Results from the various techniques indicates the presence of local structural distortions around Mn in all substituted and the concentration varied compounds. This distortion in the A-site substituted compounds depend on the packing fraction of the constituent elements in the unit cell. Further in case of transition metal substitution at Mn site, more than half filled d band elements forms phase separated compounds resulting in cluster glassy ground state.

t0018

Structural and Lithium Ion Conduction Characteristics of Lithium Sulfate Based Solid Electrolyte Systems

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The investigation of the well-known ionic conductor lithium sulfate (Li_2SO_4) provides an excellent opportunity to understand the Li^+ ion dynamics in different phases of solid electrolytes, such as polycrystalline, glass-crystal composite, glassy, polymer as well as in thin-film form. In this context, a systematic investigation has been undertaken to improve the Li^+ ion conductivity of Li_2SO_4 based solid electrolyte materials, such as the polycrystalline Li_2SO_4, quenched Li_2SO_4, glassy electrolyte mol% (100-*x*)Li_2SO_4:*x*P_2O_5, polymer electrolyte $(PVA)_n$:Li_2SO_4 and Li_2SO_4 thin film using e-beam evaporation. In this study, a multi-technique approach was used to quench Li_2SO_4 from the high-temperature melt. Fabrication of Li_2SO_4 thin films was successfully attempted by the electron beam evaporation technique and the deposition conditions were systematically optimized to get stable Li_2SO_4 thin films. All the obtained samples were systematically investigated through XRD, SEM, DSC, Raman spectroscopy, FT-IR spectroscopy, and impedance spectroscopy measurements.

t0019

Evolution Of Half-Metallicity In Antisite Disorder Controlled Full Heusler Alloy: Fe_2TiSn

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Induction of half-metallicity in an otherwise semimetallic Fe_2TiSn full Heusler system using elemental substitution has been successfully attempted in this work. The first step towards our objective was to modulate the amount of Fe/Ti anti-site disorder present in Fe_2TiSn. This was achieved through resonant X-ray diffraction measurement. The situation for half-metallicity was created in two ways: by substituting Sb at Sn site, and by substituting Cr at Ti site, in the Fe_2TiSn composition. Along with a decrease in anti-site disorder, a completely spin-polarized half-metallic ground state was realized in both the substituted compositions. We were also able to successfully explain the long-debated low-temperature anomaly in the transport property of pristine Fe_2TiSn to be a result of weak localization and the origin of magnetic correlation in the system.

t0020

Role Of Chemical Pressure In Spin-Disordered $Ho_2Ge_xTi_{2-x}O_7$ system

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Frustrated systems help to discover new states and new properties of matter. $Ho_2Ge_xTi_{2-x}O_7$ series had been synthesized through standard solid-state route. $Ho_2Ti_2O_7$ crystallizes in cubic $Fd\bar{3}m$ space group, and $Ho_2Ge_2O_7$ belongs to tetragonal $P4_12_12$ space group. The crystal lattice is bipartite consisting of two interpenetrating sublattices. $Ho_2Ti_2O_7$ and $Ho_2Ge_2O_7$ magnetically frustrated systems are important due to their exotic spin relaxation phenomenon originating from their ground state degeneracy. The role of quantum fluctuations, along with the correlations within the ground states and low-temperature spin dynamics, had been discussed in details. The effects of chemical pressure upon the band gap tenability, from insulator ($Ho_2Ge_2O_7$) to high band semiconductor ($Ho_2Ti_2O_7$) has been elaborated.

t0022

Theoretical Insights of (Un)doped TiO_2 as a Photocatalyst for Water Splitting

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TiO_2 anatase is considered to play a significant importance in energy and environmental research [1]. However, for developing efficient photocatalyst for water splitting, the major drawback is its large bandgap of 3.2 eV [1, 2]. Herein, we report using state-of-the art hybrid density functional theory and *ab initio* atomistic thermodynamics the doping of a metal and a non-metal in anatase TiO_2 [3, 4, 5]. The latter helps to capture the environmental effect that may provide theoretical guidance to experiment about the kind of defects that are thermodynamically stable at a realistic condition. We discern that the charged defects are stable in addition to neutral defects in anatase TiO_2. Our results reveal that despite the response in visible light region, the dopants in TiO_2 cannot always enhance the photocatalytic activity. This is due to either the formation of recombination centers or the large shift in the band edges. Amongst various metal and non-metal dopants, S_O in anatase TiO_2 is the most potent candidates to enhance the photocatalytic efficiency of anatase TiO_2 under the visible light irradiation.

t0023

Origin and Tuning of Some Emergent Multifunctional Properties of Selected Transition Metal Oxides

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In this paper, we highlight our investigation on some emergent multifunctional properties of selected transition metal oxides with the holistic focus of designing, synthesis and detailed experimental characterizations that have enabled us towards the controlled optimization of the desired physical properties. First, we have identified and tuned various controlling parameters which lead to the optimization of enhanced ferroelectricity and ferromagnetism (i.e. multiferroicity) at room-temperature in Bi-Fe dual-doped $BaTiO_3$ system, which is also extremely promising as alternative high-*k* dielectric materials and toward enhanced room-temperature photovoltaic effect as they provide a unique platform with the simultaneous optimization of low band gap (~1.5 eV), high ferroelectric polarization (~5 $\mu C/cm^2$) and good electrical conductivity. Subsequently, we briefly highlight how magnetic frustration helps in controlling spin-flop transition in Mn-doped $MnTiO_3$, the role of cationic disorder on the $\uparrow\uparrow\downarrow\downarrow$ magnetic ordering stability in Ca_3CoMnO_6 and on the emergence of inverse magnetocaloric effect in $Fe_{1-x}Mn_xCr_2O_4$ series. We have also identified the presence of a unique antiferromagnetism in ultra-thin strained $YTiO_3$ in a superlattice with diamagnetic $CaTiO_3$.

t0024

Fabrication and Characterization of SiO_2 Microcantilevers For Relative Humidity Sensing

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SiO_2 Microcantilevers (MCs) of various dimensions were fabricated using Direct Laser Writer and wet chemical etching methods, and were explored for ultrasensitive and ultrafast

Relative Humidity (RH) sensing. Various microfabrication process parameters such as laser dose and pre/post backing temperature to successfully release the SiO_2 MCs were optimized. As a prelude to RH sensing studies, the effect of inherent biaxial curvature on the resonance frequency and high-temperature post-release high temperature annealing on the residual stress evolution of SiO_2 MCs, were studied. RH sensing experiments were performed by measuring the shift in resonance frequency of MCs while RH is varied between 20% and 90% using Nano Vibration Analyzer. For this purpose, an air-tight chamber was indigenously designed and calibrated in the entire RH range. It is shown that the introduction of controlled micro-patterns on the MC surface can enhance the RH sensitivity of these devices without compromising other sensor characteristics such as response/recovery times and hysteresis. Finally, real-time monitoring of human respiration during normal and slow inhale/exhale breathing cycles using micro-patterned MCs is demonstrated.

t0025

The Many Facets Of Noise: Effects In Classical And Quantum Statistical Systems

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We discuss how noise impacts the static and dynamic properties of a spectrum of representative classical and quantum systems. For a paradigmatic noisy model of spontaneous synchronization, we show by obtaining exact results that the autocorrelation of the order parameter in the nonequilibrium steady state decays exponentially with a rate that increases with the noise strength. For a nonlinear dynamical system, we show using a path-integral approach how one may obtain its bifurcation behavior from the corresponding noisy dynamics in the weak-noise limit. For mean-field classical Heisenberg spins, we unveil within deterministic dynamics the full range of size-dependent quasistationary behavior observed during relaxation to equilibrium and that the corresponding noisy dynamics exhibits a size-independent faster relaxation. We also obtain using a dynamical approach the critical exponents describing power-law behavior of response to a field and show how they differ significantly from those obtained from static phase-space distribution. For model quantum systems subject to random projective measurements evolving in discrete and continuous time, we obtain universal decay laws for the mean survival probability of an initial state.

t0028

Nanostructured $NaMnPO_4$ Based Supercapacitors - Electrochemical Performances under Ambient and Non-Ambient Conditions

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The growing understanding and expertise to develop novel nanoparticles ranging from solid, hierarchical to hollow, has allowed the resurgence of Na-ion based energy storage systems. In this thesis work, a successful synthesis strategy to obtain single phase $NaMnPO_4$ is established. It is shown that $NaMnPO_4$ can be used as an effective electrode material for Na-ion supercapacitors, with specific capacitance values that are comparable or higher than those reported in literature pertaining to such materials. To induce a quantum jump in the specific capacitance value, a strategy based on the use of redox additive modified electrolytes is proposed. Further, the electrochemical studies under various external factors like: temperature and external magnetic field has been investigated. A new theoretical model is proposed for the first time to explain the magnetic supercapacitors.

t0029

Magnetic and Structural Properties of Transition Metal Nitride Thin Films

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In this thesis work, the structural and magnetic properties of Fe_4N and Co_4N thin films have been studied for their phase formation, film-substrate interdiffusion, and thermal stability. These compounds belong to the metal-rich category of transition metal nitrides and have been explored for their magnetic, electrocatalytic, and transport properties. Co_4N has found its usage as a bifunctional electrocatalyst in metal-air battery electrodes and water splitting reactions, while Fe_4N is predicted to be an ideal candidate in magnetic tunnel junctions. Both of these compounds have been found to possess a high saturation magnetization and spin polarization ratio, however, there are discrepancies in theoretical prediction and experimental results. Such discrepancies could arise due to various reasons such as phase purity, method of deposition, substrate temperature, etc. In this thesis, we have addressed these issues and found that substrate-film interface and growth condition play a pivotal role in determining the properties of Fe_4N and Co_4N thin films. One of the novelties of this thesis is to combine lab-based techniques with synchrotron and neutron-based techniques to gather further insight about these discrepancies correlating structure and magnetization of these compounds.

t0030

Phase Transformations and Structure-Property Correlations in Ni-Cr-Mo alloys

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In view of potential applications of Ni-Cr-Mo alloys in high temperature environments, particularly, in molten salt nuclear reactors, the effect of Cr substitution in the Ni-Mo alloy (Mo+Cr content~ 20 at.%; Ni-16 wt.% Mo-7 wt.% Cr alloy) was studied using X-ray absorption spectroscopy, electron microscopy and the first principles estimation of multisite interaction energies between the constituent atoms. Electron microscopic investigations reveal that Cr addition leads to suppression of long range ordered precipitate of $D1_a$ type (BCT, I4/m) as opposed to the case of binary Ni-20 at.% Mo alloy indicating that Cr plays a crucial role in altering the nearest neighbour interaction energies, which finally dictate the ordering tendencies in these alloys. Rigorous extended X-ray absorption fine structure studies on Ni-Mo and Ni-Cr-Mo alloys establish that Cr replaces Mo in the fcc lattice and preferentially bonds with Ni in the first coordination shell thereby stabilizing the disordered fcc phase over the $D1_a$ phase. The mechanisms of microstructural degradation of Ni-Mo-Cr alloy when exposed to oxygen containing FLiNaK (candidate coolant) salt as well as chemical interaction with simulated fission product tellurium was also established. The study provided insights to understanding the phase transformation mechanisms as well as the microstructural stabilities of the selected alloy under simulated reactor environment and finally concluding that it possesses favourable properties as a structural material.

t0031

Investigation Of Magnetic Transitions In Some RT2X2 Type Rare Earth Intermetallics

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The work presented in thesis is based on the investigation of magnetic transitions of RT_2X_2 intermetallic compounds exhibiting multifunctional properties and quantum critical phenomena in heavy fermion Ce based intermetallic compounds. The study serves as a reference work to rare earth and transition metal based intermetallic compounds comprising of two magnetic sublattices as well as Ce based heavy fermion compounds.

t0032
Synthesis and Characterization of $CoSb_3$ Based Materials for Mid-Temperature Thermoelectric Applications
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Thermoelectric is the technology for clean power generation, in which waste heat is directly converted into electricity. Current work explores possibility of enhancing the TE performance of rare-earth-free $CoSb_3$-based materials employing a doping approach. A fast and facile route of arc melting and spark plasma sintering is adopted for synthesis. Further, suitable dopants have been used to achieve high TE performance in p and n-type $CoSb_3$ based materials. After successful optimization of efficient p-and n-type $CoSb_3$ based compositions, TE elements (single legs) were fabricated with suitable metallization and characterized for device performance parameters.

t0036
Density Functional Theory of Free and Oxide Supported Metal Nanoclusters and Nanoalloys: A Heterogeneous Catalysis
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The proposed work initiated to study the atomic and electronic structure of free and oxide supported nanoclusters (NCs) and nanoalloys (NAs) to understand their morphology, bonding configurations and modified electronic plus vibrational properties in order to explore their catalytic activity with two principal objectives in mind: (1) design and study oxidation of carbon monoxide (CO) over free and oxide supported NCs/NAs to avoid the deactivation of the catalyst by CO and (2) to study the pure and bimetallic NCs for the reduction of carbon dioxide (CO_2) into sustainable carbon-based fuels. Our findings offer an efficient strategy for precise alloying of NCs which promotes the development of a highly efficient and active catalyst.

t0037
Advanced Electrodes From 2D Layered Materials For Li^+ and Na^+ Storage
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Two-dimensional (2D) materials with large surface areas, high charge-carrier mobility, and unique chemical and electronic properties are finding applications in various fields including energy-storage applications. These materials are promising candidates in rechargeable batteries to fulfill the demands for superior rate performance, long cycle life, and higher power and energy density requirements. As a part of this objective, we have studied a new class of bulk semiconducting transition metal dichalcogenides (TMDs), specifically, the 2D layered structure molybdenum ditelluride ($MoTe_2$). The relatively high interlayer spacing of $MoTe_2$ about 0.70 nm (graphite (0.335 nm) and MoS_2 (0.615 nm)) and the higher electronic conductivity of $MoTe_2$ make it an efficient anode material for both lithium and sodium-ion batteries (SIBs); the risk of substantial volume change is also absent in $MoTe_2$. We studied both 2H and 1T' phases of molybdenum ditelluride ($MoTe_2$), which was synthesized through a facile solid-state reaction route synthesis process. We have further investigated the lithium and sodium storage mechanism in both 2H and 1T' phases of $MoTe_2$ during the Li^+/Na^+ insertion and desertion process by using different Synchrotron-based in situ/ex situ experimental techniques alongside theoretical studies.

t0039

Electronic structure and morphology of Manganese based alloys and thin films

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Here, we have shown the important of different forms of photoemission spectroscopy to study various classes of materials. In Mn based Heusler alloys, the origin of modulation in the martensite phase has been investigated, which has been associated with the charge density wave formation. The study of bulk electronic structure of $CeMnNi_4$ discusses the origin of its high spin polarization value, where electron-electron correlation and anti-site disorder play important roles. This paper also deals with the surface electronic structure and morphology of epitaxial thin film of Au-Sn, where we show the existence of graphene-like novel band structure in a specific surface alloy phase by using angle resolved photoemission spectroscopy (ARPES). In addition, here, we have studied the surface electronic structure of different Au-Sn compounds grown in situ by thick layer of Sn deposition on Au(111) substrate at various temperatures. ARPES has been also used to probe the 3D band structure of Ni_2MnGa(100) surface.

t0041

Structure, Dielectric Property and Cation Dynamics In $MA_{1-y}FA_yPbX_3$ (X = I, Br) Perovskites

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Hybrid Organic-Inorganic Lead Halide Perovskites (HOIP) are represented by $APbX_3$, where A is the organic cation e.g. MA ($(CH_3NH_3)^+$) or FA ($(CH(NH_2)_2)^+$), X is halide anion. We have investigated dielectric properties of the solid solution series, $MA_{1-y}FA_yPbI_3$ for various compositions with $1 \geq y \geq 0$. Through temperature dependent single-crystal and powder XRD, we could establish a structural phase diagram for these solid solutions. Most interesting finding in this system is that, structure and dielectric property are strongly correlated. To understand the dynamical nature of these two cations, namely MA^+ and FA^+ in $APbBr_3$ system, we have performed quasi elastic neutron scattering (QENS) experiments. We could

establish that MA^+ exhibits 3-fold rotation around C-N axis and 4-fold jump rotation about C-N axis itself, in low-temperature orthorhombic and high-temperature tetragonal/cubic phase, respectively. In contrast, FA^+ exhibits an isotropic motion throughout all the temperature range covering orthorhombic-tetragonal-cubic phases. Thus, through QENS experiments, we could realise the contrasting nature of these two cations. We report results of our structural investigation of the impact of pressure on $MA_{1-y}FA_yPbI_3$ with $1 \geq y \geq 0$.

t0042

Growth and application of low-dimensional SnO_2

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Tin oxide (SnO_2) is technically an *n*-type semiconductor with a wide bandgap (~ 3.67 eV RT) and high exciton binding energy (130 meV). Synthesizing SnO_2 in nanostructures (NSs) comes with the privilege of decorating various defects. More importantly, the presence of defects like in-plane oxygen vacancy (V_P) and bridging oxygen vacancy (V_B) in SnO_2 fetches scientific curiosity and opens up the door for many technical utilities. Though rigorous experimental and theoretical attempts have been made to allocate defect distribution in NSs, the detailed modeling and absolute correlation with various applications need further understanding. This thesis program is based on evaluating defects in 0-D and1-D SnO_2 NSs and effective utilization of these defects in applications like resistive and optical-based gas sensing, supercapacitor, dielectric, and photocatalytic properties. 1-D SnO_2 NSs for waveguide application is also demonstrated. For the growth of these NSs, both chemical route and chemical vapor deposition (CVD) techniques have been followed. For morphological and structural characterization, XRD, TEM, FESEM, Raman, photoluminescence, FTIR, XPS, EELS, Mossbauer, and XAS spectroscopy are carried out.

t0043

Study of the Thermoelectric Properties of $R_xCo_4Sb_{12}$ (R=In, Ba) with InSb/GaSb Nano Inclusions

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The Co_4Sb_{12} based skutterudite materials are the widely explored thermoelectric (TE) materials for mid-temperature applications. But the high lattice thermal conductivity (κ_L) of these materials leads to a low figure of merit (zT). Filling the voids of cage forming compounds by electropositive elements and homogeneous distribution of nano-sized secondary phases in the bulk matrix are promising approaches to enhance zT of these materials. These two approaches were combined by filling elements R (= In, Ba) into the void of Co_4Sb_{12} and dispersing InSb/GaSb nanoparticles in the bulk matrix of $R_xCo_4Sb_{12}$. The fillers (In^{+1} and Ba^{+2}) in the void donated their outermost electron to Co_4Sb_{12}, resulting in a significant decrease in ρ. The fillers, being loosely bound to the surrounding of Sb atoms, rattled inside the oversized voids and reduced κ_L by enhancing phonon scattering. The dispersion of InSb/GaSb nanoparticles reduced κ_L further due to the enhanced interface scattering of phonons, which resulted in the highest zT~1.4 for the $(InSb)_{0.15} + Ba_{0.3}Co_4Sb_{12}$ and $(GaSb)_{0.1} + In_{0.2}Co_4Sb_{12}$ nanocomposites at 773 K. The results obtained in the thesis provides a better understanding of the combined approaches to tune the properties of TE materials

t0044

Structural and Electronic Transport Properties of 3D Topological Insulators

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High quality and phase pure Bi_2Te_3, $Pb_2Bi_2Te_3$, $PbBi_{2-x}Fe_xTe_4$ (x = 0, 0.025 and 0.05), $SnBi_2Te_4$, $PbBi_4Te_7$, $Bi_{2-x}Sb_xTe_{3-y}Se_y$ (BSTS), In- and Sn-doped BSTS single crystals were grown through modified Bridgeman technique. Electronic transport measurements were carried out on bulk single crystals and nano devices to explore their non-trivial topological surface states (TSSs) with π-Berry phase. Comparative Fermiology study of TSSs for $(Sn/Pb)Bi_2Te_4$ reveal TSSs in $PbBi_2Te_4$ are of superior quality over the TSSs in $SnBi_2Te_4$. The analysis of the Shubnikov-de Haas (SdH) oscillation reveals the linear Dirac dispersion nature of the TSSs in Fe-substituted $PbBi_2Te_4$. The double Dirac cone assisted surface states transport in $PbBi_4Te_7$ single crystal and nano device are explored from electronic transport measurement. Determined *g*-factor from peak splitting in SdH oscillation corroborate strong spin–orbit coupling of surface Dirac Fermions in $PbBi_4Te_7$ single crystal. Moreover, 2D unusual conductance fluctuations are identified in magnetotransport measurements of $PbBi_4Te_7$ nano device. Bulk insulating nature and evidence of conducting surface states for In- and Sn-doped BSTS single crystals are revealed from electronic transport measurements.

t0045

First Principles Characterization of Metal Nanowires for Sensing and Energy Harvesting Application

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Today, we are living in a world of ever increasing energy hungry population. Energy, as fuel or power, has become a fundamental piece of endurance and progress. In this advancement, we have started facing various environmental issues, such as air pollution, sea acidification, greenhouse effect and many more to come in future. Concerning with these problems, we were motivated to study the applications of metallic nanowires for sensing and energy harvesting. Our work is mainly focused on the study of gas sensing and thermoelectric properties of different metallic nanowires. We have worked on transition metal based metallic nanowires (PdP_2, $PdAs_2$ and VO_2), Si and Ge based metal core/shell nanowires for different applications and different monoatomic nanowires (Al, B, As, Sb-NW).

t0046

Investigation Of Correlated Electron Systems Including Materials With Complex Magnetic Structures

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The work carried out in the thesis tried to encapsulate the study of electron correlations and non-trivial magnetic structures in 3*d* and 4*f* electron based non-centrosymmetric compounds. The work focused on identifying new systems hosting skyrmions which are hedgehog-like structures of magnetic spins and the doping induced quantum phase transitions (QPTs).

t0047

Insights into the Surface Chemistry of Adsorption of CO_2 and NO_2 Molecules on TiO_2

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The electronic structure, be it at the interface of molecules with surface gives rise to unusual physical and chemical properties which finds applications in the area of electrochemistry, photocatalysis, and heterogeneous catalysis. The atomic simulations provide key insights into the reaction energetics and kinetics. In the present work, we have examined the adsorption mechanism of molecules such as CO_2 and NO_2 on TiO_2 surface followed by their co-adsorption with H_2O and subsequent conversion process. A three-state quantum mechanical model is proposed to explain the charge transfer mechanism which will have universal appeal to the surface-molecule interaction. Utilizing this model, a step selective reactivity order among low-index facets of anatase TiO_2 is established, and the change in exchange-correlation energy before and after adsorption is proposed as an indicator for adsorption strength. Extending the analysis to NO_2, which have bent geometry we have formulated the chemical conversion pathway to useful products such as HNO_2 and HNO_3.

t0053

Synthesis, Characterizations and Physical Properties of Perovskite Oxide and Oxynitride: An Investigation by Synchrotron-based Techniques

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This report focuses on the SrTiO3 (STO) and possible enhancement in dye degradation efficiency of a photocatalytic material for the elimination of pollutants present in water and to study their structural and optical properties. Correlations of these properties with the electronic structure of STO were investigated using synchrotron-based techniques. The photocatalytic degradation of methylene blue dye using ball-milled STO powders is studied and observed that the particle size of STO decreases after increasing the time of ball-milling. The evolution of optical blue-green emission in STO thin films implanted by 100 keV nitrogen ions at different ion fluences is reported where the modification in local surroundings of Ti ions results in the alterations of its coordination geometry and valency. The bandgap engineering of STO films with swift heavy Ag ions is studied and reported that an appropriate fluence of Ag ion beam results in the bandgap of STO close to the visible light necessary for several applications. N ion implanted STO single-crystals were studied by synchrotron X-ray Nano Diffraction and angle dependent XAS, and confirmed the formation of STO based oxynitride.

t0055

Development of Carrier Selective Contacts and Upconversion Phosphors for Silicon Solar Cells

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In this work we demonstrate various ways – using state of art technology - carrier selective contacts and upconversion phosphors, to improve the performance of c-Si solar cells. Initially, hybrid organic/Si heterojunction solar cells, with PEDOT:PSS and PEDOT:PSS-CNT composites are investigated as hole selective layers (HSL), where the advantages of organic and inorganic materials are combined. PEDOT:PSS/Si solar cell with SiO_x passivation layer and back surface field (BSF), achieved an efficiency (η) of 9.78%, while the, PEDOT: PSS-CNT/Si solar cell with optimized CNT concentration obtained an η of 9.05%. Further, novel p-type transparent boron-doped copper oxide (Cu_2O:B) and n-type molybdenum oxide (MoO_3) as hole selective layer deposited by industry friendly rf-sputtering and thermal evaporation method, respectively are investigated for solar cell application. The quantitative prediction of the band structure is made combining UV-VIS-NIR, XPS, and UPS measurements. Dopant free double heterojunction solar cells are fabricated using hole selective MoO_3 and electron selective MgF_2 deposited by thermal evaporation technique. Finally, spectral matching using upconversion phosphors is demonstrated as a proof of concept. Yttrium based upconversion phosphors are synthesized by simple method and the host dependent luminescence properties are investigated and studied. The UC phosphors are incorporated into an a-Si:H and the solar cell and the performance is studied systematically. A 7.5 % improvement in J_{sc} is obtained for the a-Si:H solar cell incorporated with YF_3: Yb^{3+}/Er^{3+}. These results provide better understanding of various carrier selective contacts and able to report for the first time novel Cu_2O:B HSL.

t0056

Investigation Of Temperature And Frequency Dependent Electrical Transport Phenomena At The Interface Of Bilayered Ferromagnetic – Ferroelectric Thin Films And Related Issues

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This thesis contributes to a comprehensive study of electrical transport through FM-FE interface of complex oxides focusing on the low symmetry FE phases of FE $BaTiO_3$ (BTO) as well as the negative spin polarization of FM $SrRuO_3$ (SRO) that has not been reported before. We use the temperature and electric bias dependent transport in the FE layer containing multilayer devices to explore such issues like effects of phase transition in BTO on Schottky barriers as it is cooled below the ferroelectric transition temperature, control and modulation of Schottky barriers formed at interfaces with BTO which can be a n-type semiconductor, aspects of spin polarized transport when the FM layer SRO is a minority band ferromagnet and last but not the least the effect of oxygen stoichiometry of the BTO layer on the junction transport.

t0057

High Performance Optical and Gas Sensors Based on 2D/3D Heterostructures

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In my thesis work, I have extensively studied the exciting physics of 2D/3D heterostructures. To understand the suitable application of different heterostructures, we have studied the band

alignments at the heterointerfaces. We have measured the conduction and valance band offsets across the 2D/3D heterojunctions by using X-ray and Ultraviolet photoelectron spectroscopy techniques. Interestingly, the obtained alignments was found to be useful particularly for designing broadband optoelectronic devices. Hence, we have demonstrated the photo-sensing applications of 2D/3D heterostructures. I have also studied the carrier dynamics across the heterojunctions to give an insight into different scattering mechanisms. To check the suitability of our device for multifunctional operations, I have evaluated the gas sensing performance of my heterostructure based devices. We have achieved ultrahigh sensitivity, excellent selectivity, and quick detection of different gas molecules at a very low operating power due to large surface area provided by the 2D materials. Upon gas exposure, the molecular adsorption tuned the barrier height at the heterointerface hence a high sensitivity was observed. Therefore, a single device could be used for multifunctional applications.

YOUNG ACHEIVER AWARD NOMINEE'S PAPERS

y0002

Optically Multifunctional Nanomaterials

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The present work presents the design, development and application of efficient, bright, photostable, biocompatible, etc. nanomaterials for application in solid state lighting, x-ray scintillators, high pressure luminescence, afterglow phosphors, nuclear waste hosts, etc. Doped Spinel based materials showed very efficient persistent luminescence for a very long time and further improvement was achieved by thermal treatment, core-shell strategy, etc. Pyrochlore materials showed high pressure induced tunable luminescence and structural phase transition induced evolution of new luminescent centres. The similar materials demonstrated excellent feasibility as nuclear waste hosts with high efficacy for actinide doping and gamma irradiation induced structural phase transition. Our nanomaterials also performed exceedingly well as x-ray scintillators by converting energetic x-ray into visible photons and further demonstrated phase transition induced tunable radioluminescence. We could achieve light emission from near ultraviolet to 2.8 micron in LaF_3:Yb,Er. We could also design optical based thermal, pressure and food spoilage sensors. We believe our work will have farfetched influence in the novel functionality in design aspects of multifunctional phosphors.

y0003

Mesoporous MnO_2@NTO Core-shell Heteroarchitecture for High Performance Energy Storage Electrodes

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The problem of the low energy density of pseudocapacitors can be effectively addressed using novel core-shell heterostructured electrodes. Here we report the hydrothermal synthesis of the core-shell structure of 2D MnO_2 nanoflakes and 1D mesoporous $NiTiO_3$ rods as an efficient electrode material for supercapacitor. The MnO_2@NTO core-shell heterostructure provided a larger surface area and more pathways for the diffusion of OH^- ions. The MnO_2@NTO showed specific capacitance of 1054.7 F/g, specific energy of 15.7 Wh/kg, and specific power of 1822.8 W/kg, which is fairly significant than the core-shell nanostructures of $NiCo_2O_4$/MnO_2, PEDOT/MnO_2, graphene/MnO_2, MnO_2/CNTs, and PU-NCNT/MnO_2 composite, etc.

y0004

Superconducting Properties of Re_6Mo

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Re-based superconductors recently emerge as a new family of unconventional superconductors. However, the role of crystal structure and Re is not clearly understood. In this regard, Re_6Mo is the best candidate as it crystallizes in a centrosymmetric structure in contrast to its iso-compositional non-centrosymmetric compounds, Re_6X (X = Zr, Hf, Ti). Here, we systematically investigate the normal and superconducting properties Re_6Mo alloy using magnetization, heat capacity, and resistivity measurements. Detailed studies suggest Re_6Mo is a type-II moderately coupled s-wave superconductor.

y0005

Formation Of Hydrogen Bonded Liquid Crystals Between Benzoic Acids

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Hydrogen bonded liquid crystals a special branch of thermotropic liquid crystals finds wide interest among the scientists due to their ease formation of the mesogenic phases and the applicational aspects so far examined. This liquid crystalline mesogenic phase is an intermediate state that exists between crystalline solid and amorphous liquid. Physico-chemical investigations in self- assembled hydrogen bonded liquid crystals formed between p-n alkyloxy benzoic acids is discussed in the present discussion. Chemical, spectral, optical, thermal, electrical and dielectrical properties of the formed mesogens are discussed in detail.

y0007

Discovery of Bain Distorted Premartensite Phase in Pt Substituted Ni_2MnGa Magnetic Shape Memory Heusler Alloys

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Magnetic shape memory Heusler alloys (MSMHAs) have generated tremendous interest in recent past due to their large magnetic field induced strain (MFIS) in the low-temperature martensite phase. In MSMHAs the stoichiometric Ni_2MnGa has been investigated intensively due to its large (10%) MFIS. Ni_2MnGa exhibits paramagnetic to ferromagnetic transition at temperatures Tc ~373 K and martensite transition at temperature T_M ~ 210 K, respectively. The martensitic transition in Ni_2MnGa is preceded by a precursor (premartensite) phase transition around T_{PM}~260 K. The large MFIS of Ni_2MnGa is also closely linked with the incommensurate modulated structure of the martensite phase. As the modulated phase of Ni_2MnGa appears through a modulated premartensite phase and not directly from the high temperature austenite phase, understanding the premartensite phase and its effect on the low temperature martensite phase transition has been a hot topic of research in recent years. We present here direct evidence for the robust Bain distortion of the premartensite phase in Ni_2MnGa MSMHA substituted with 10% Pt through a high-resolution synchrotron x-ray powder diffraction study.

y0008

Primary and secondary charge transfer interaction of Metal Phthalocyanines with adsorbed target analytes

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Better selectivity and sensitivity of Metal Phthalocyanines (MPcs) under ambient conditions allows their utilization as chemresistors for the detection of toxic gases in environment and explosive detectors to control terrorism activities. Flexibility of MPcs to replace central metal ions, ease of substitution with different functional groups and variations in their resistances with exposure of reducing, oxidizing and other volatile gases allow their versatile applications. In the present work, we aim to integrate the advantages of three MPcs with three different metal ions, similar functional group and a ligand attached to central metal ion to device a sensor. The fabricated sensors have been observed to have amended properties with

better response-recovery times, sensitivity, selectivity and stability as compared to individual counterparts. Four Chemresistor devices were fabricates using permutation combinations of three MPcs namely; tetrasulfonic acid tetrasodium salt functionalized Nickel Phthalocyanine (NiPcS) and Copper Phtalocyanines (CuPcS) and Aluminum Phthalocyanine hydroxide (AlPcOH). For benzene, NiPcS-AlPcOH composite exhibited maximum sensitivity (≈ 2.73 ppm^{-1}) and for bromine, CuPcS-AlPcOH composite shows highest sensitivity (≈ 73 ppm^{-1}).

y0010

Ce(IV) Intercalated And Nano Ceria Incorporated Titanate Nanotubes For Treatment Of Anionic And Cationic Contaminants In Water

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The current study presents a versatile material Ce (IV) intercalated and nano ceria incorporated titanate nanotubes (CCTNT) that efficiently removes both cationic and anionic contaminants from water. Water remediation is the need of the hour as the presence of various contaminants in water is a global problem. It is rare that a single material successfully removes both cationic and anionic contaminants from water. The material is synthesized by a two-step wet chemical route. XRD proves the presence of monoclinic titanate and cubic ceria phase in CCTNT. TEM images confirmed the morphology to be nanotubes decorated with ceria nanoparticles. It also possesses a high surface area of 210 m2/g with mesoporous nature as confirmed by BET. Both these properties along with the stability of structure of the material enabled its application for water remediation. CCTNT could remove 91% of fluoride and 95% of lead ions from contaminated water with 10 mg/L of fluoride and lead ions respectively, in a short span of 30 minutes.

y0011

Exploring Optical Properties in Perovskites-Based Solar Cells from Many-body Perturbation Theory

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Materials for optoelectronic applications have received a lot of attention worldwide in a variety of fields over the past several decades. Understanding these materials at the theoretical perspective is never been easy because of the exchange-correlation functional that needs to be carefully analyzed in the light of electron's self-interaction error and spin-orbit coupling (SOC). Conventional first principles-based simulation under the framework of Density Functional Theory (DFT) with local/semi-local functionals (viz. LDA or GGA), is not sufficient to determine the excited state properties. Therefore, to study the excited state properties of potential photovoltaic materials, we employ a general framework of the first-principles calculation under many-body perturbation theory approach (GW/BSE) [1]. Some of the findings of different class of materials are discussed here. For example, to reduce Pb-toxicity from lead halide perovskites, we find significant degradation of optical properties and solar cell efficiency on more than 50% substitution of Sn in place of Pb [2, 3]. Thus as an alternative to lead halide perovskites, we have explored environment friendly double perovskites and their derivatives obtained by doing sublattice mixing via high-throughput screening [4-5]. Unfortunately, we find apart from a few promising ones, most of the conformers obtained via sublattice mixing suffer from stability issues [4-6]. This motivates us to explore a different class of materials viz. chalcogenide perovskites as they are earth abundant, environment friendly, stable and exhibit optimal optical response [7]. We have

studied the optical and excitonic properties of bulk as well as Ruddlesden-Popper (RP) phases of chalcogenide perovskites that show enough promise as an evolving class of upcoming optoelectronic materials, especially in solar cells [8].

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y0012

Hydrothermal Synthesis of mesoporous $ZnCo_2O_4$ For Supercapacitor Application

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In present study, mesoporous $ZnCo_2O_4$ nanostructure was synthesized by hydrothermal method followed by annealing treatment. The formation of $ZnCo_2O_4$ was confirmed by X-ray diffraction (XRD) and Fourier Transform infrared spectroscopy (FT-IR) study. The Field emission scanning electron microscopy (FESEM) study revealed the formation of mesoporous $ZnCo_2O_4$ nanostructures. The energy dispersive X-ray spectroscopy (EDS) study also confirmed the formation of $ZnCo_2O_4$. The as prepared $ZnCo_2O_4$ electrode exhibited a maximum specific capacitance of 307.9 F g^{-1} at a scan rate of 10 mV s^{-1}. The electrochemical supercapacitor study indicates the mesoporous $ZnCo_2O_4$ is a promising electrode material for supercapacitor.

y0013

Polymorphism and tunable functional properties of Rare earth Indates ($REInO_3$)

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Rare earth Indates ($REInO_3$) belong to one of the scarcely investigated interesting class of compounds exhibiting varieties of structures. In this report, an overview of our studies on polymorphism and dielectric properties are presented. A careful and controlled synthesis under different condition has been carried out to stabilize different polymorphs of $REInO_3$. Profound effect of temperature and composition on the formation phases has been revealed. A-site and B-site substitution has been carried out to understand their effect on structure and electrical properties, which lead to a mode for tuning their dielectric properties. High pressure studies on hexagonal $YInO_3$ and cubic $YbInO_3$ has also been carried out and discussed.

y0014

Static And Alternating Magnetic Field Induced Phenomena In Magnetic Nanofluids And Nanoemulsions: Hyperthermia, Force Spectroscopy and Optical Sensors For Defect Detection

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Magnetic nanofluids are stable dispersions of superparamagnetic nanoparticles in a suitable carrier fluid. In the presence of an external static magnetic field, magnetic nanofluids undergo disorder-to-order transition forming linear chain like structures giving rise to unique field-tunable optical and magnetic properties which are exploited for developing various sensors. On exposure to white light, Bragg reflection peaks are observed, when the incident wavelength matches with the periodic spacing exploiting which, weak inter-molecular force measurement is possible through the magnetic chaining technique. When subjected to a high frequency alternating magnetic field, magnetic nanofluids generate heat due to inherent Neel-Brown relaxation losses. This phenomenon is known as magnetic fluid hyperthermia and is being developed as an alternate cancer therapy due to the possibility of localized heating assisted therapeutic benefits without significant damage to the surrounding healthy cells. This article discusses a few research activities on magnetic nanofluids and nanoemulsions for the above-mentioned applications.

y0016

Experimental And Theoretical Investigation of Phases And Energy Profiles of Different Lattice Structures of Surfactants-DNA Complexes

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Surfactants (DTAB and MTAB) along with DNA form complex structures in aqueous media by arranging in self-assembled fashion. Small angle X-ray scattering technique reveals the structures of surfactants-DNA complexes, which acquire hexagonal phase in presence of small amount of DTAB (wt %) but for large amount of MTAB (wt %) in aqueous media for both relative concentration ratios, ([MTAB] + [DTAB])/[DNA]= ρ), 1 and 5. Structures undergo a phase transition due to an influence of NaCl salt. The structures enter a super hexagonal phase in presence of an increasing amount of DTAB (wt %) in 300 mM NaCl solutions for ρ 1. The structures gradually obtain a square phase for increasing the amount of DTAB (wt %) in 300 mM NaCl solutions with ρ 5. Theoretical calculations of energy profiles for different complex structures, which show that hexagonal phase exists for bigger micellar radius whereas square phase exists for smaller micellar radius in presence of comparatively rigid DNA of radius 1.25 nm, also explain the stability of the structures in different regimes of the micellar radius. The hexagon and square phases share the same energy state for the micellar radius of 1.1 nm in a monovalent electrolyte solution for κ=2 nm.

y0019

Anharmonic atomic dynamics in energy materials

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The quest for advanced materials with desired properties requires understanding their complex atomic dynamics. The atomic dynamics in the superionic, thermoelectric, and negative thermal expansion are very anharmonic and play a critical role in controlling their thermodynamics and transport properties. Here, we combine extensive neutron scattering measurements and atomistic modeling to unravel the role of atomic dynamics in the transport and thermodynamic properties of superionic and negative thermal expansion compounds. The studies on Li/Na-based superionic conductors provide insight into the correlation between diffusion and host dynamics. We have investigated the role of host-flexibility, vacancies, and amorphization on phonon spectrum and identified important dynamical

descriptors to screen the potential solid-electrolytes. Our extensive studies on a variety of negative thermal expansion materials (MOF, cyanides, and oxides) provide a critical understanding of the nature of anharmonicity and thermal expansion behavior. Besides this, we performed a Monte-Carlo simulation to design and optimized the components of an upcoming neutron spectrometer at Dhruva to covers the more extensive dynamical range with better energy resolution.

y0020

Investigating quasi-particle coupling in momentum-energy and space-time domain

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Quasi-particle (QP) coupling -- phonon-phonon, electron-phonon, magnon-phonon -- underpins a wide range of properties in technologically important materials, such as superconductors, thermoelectrics, multiferroics, topological insulators (TIs). Yet, their direct measurements and simulations remain challenging. Here I describe our experimental and theoretical efforts to investigate QP coupling in the momentum-energy (**Q**-*E*) and real space-time (**x**-*t*) domain providing a complementary understanding of the origin of QP coupling. Our studies have led to the discovery of multiple Kohn anomalies in Uranium metal at room temperature, origin of phonon-phonon coupling driven hybrid improper ferroelectric $SrBi_2Nb_2O_9$, weak magnon-phonon coupling in biferroic $YCrO_3$, and time evolution of phonon-phonon coupling driven thermal transport in nanostructured Silicon. These results enhance our fundamental understanding and provide focused guidance on the controlled tweaking of QPs for solving rapidly evolving technological challenges.

y0024

Improved Behavior of Ni Substituted ZrCo Nanoclusters for Hydrogen Storage: A First Principles Study

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Zirconium-Cobalt alloy has been proposed as a storage material for hydrogen isotopes in storage, delivery and supply (SDS) systems of ITER. Hydrides of Ni-substituted ZrCo alloy has been found to possess improved anti-disproportionation property and suitable to overcome the drawback of ZrCo alloy. Here, the structural, energetics and electronic structure of Ni substituted ZrCo nanoclusters and their changes upon hydrogenation has been studied using DFT based first-principles method. The lowest energy structure of bare and Ni-substituted ZrCo nanoclusters were established. It is observed that those have comparable binding energies while unsubstituted clusters are more stable than the Ni-substituted one, but in case of H-atom adsorbed clusters, it is opposite. The lower binding energy of Ni-substituted ZrCo clusters indicates its vulnerability towards hydrogenation reaction. Ni has been found to be an active site for hydrogen adsorption and facilitate to increase the gravimetric capacity of the alloy. The nature of chemical bonding of these clusters and with their H-adsorbed counter parts has been depicted in terms of charge density distribution.

y0025

Plasma Functionalized Vertical Graphene Electrodes for Supercapacitor Applications

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Recently, the vertical graphene nanosheets (VGN) is emerged as potential electrode material for supercapacitors, due to their intriguing properties. It's unique 3D interconnected porous networked geometry, bestows a large surface area and high density of sharp edges with non-stacking morphology offers an easy access to its surface, is a big boon for its utilization as supercapacitor electrode. Herein, plasma surface functionalization is adopted to engineer the surface chemistry and in-turn to achieve super-wetting VGN's. Further, the plasma functionalization is found to manipulate the defect density and also controls the defect type (sp3 or vacancy). Additionally, the plasma functionalized VGN's exhibits one order enhancement in electrochemical capacitance with higher capacitance signifies their potentiality. Further, the spin polarized first principle density functional theory based calculations substantiated the annihilation of vacancy defects and an enhancement in sp^3 type defect depending on the type of plasma used. A solid-state supercapacitor device of supper-wetting VGN's is fabricated and demonstrated its performance by lighting an LED.

y0027

Unusual Metallic Behavior at Low Temperature, High Pressure, Thermoelectric Studies of δ – Ag_4SSe and TlSe Single Crystals

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Silver chalcogenide based superionic conductors possess liquid-like ionic diffusivity (10^{-3} $(\Omega.Cm)^{-1}$) which causes the variety of interesting physical properties such as, electronic topological transitions, metallization, and the possible emergence of superconductivity under pressure have attracted attention in recent years. Among these chalcogenides Ag_2S - Ag_2Se solid solutions have been thoroughly investigated for several decades, due to many interesting high temperature optical, electrical, and thermoelectric properties exhibited. In this connection, we discuss our recent discoveries on Ag_4SSe and TlSe single crystal structural, high pressure structure, electronic, magnetic and thermoelectric properties. The superionic electrical conductor Ag_4SSe is reported to undergo an unusual first-order structural phase transition at ~260 K with concomitant anomalous electronic properties. The diamagnetic magnetic susceptibility is of larger magnitude δ phase than in α-Ag_4SSe. Synchrotron based angle dispersive X-ray diffraction performed on aguilarite - Ag_4SeS, up to ~20 GPa to probe its high pressure structural phase transitions. Also, we discovered ultralow thermal conductivity in TlSe single crystal due to inherent Tl^+ rattling.

y0028

Insulator to metal transition in vanadium oxides

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Insulator to metal transitions (IMT) in vanadium sesquioxide (V_2O_3, T_c ~ 155 K) and vanadium dioxide (VO_2, T_c ~ 340 K) have intrigued the condensed matter physicists for

several decades. First order IMT in these have been prototypical playground for condensed matter theorists as well as experimentalists. Near room temperature IMT in VO_2 (at ~ 340 K) has been especially attractive because concurrent with IMT it also exhibits spectacular switching in transmittance/reflectance of the IR (infrared) radiations which makes it potentially useful for designing thermochromic smart windows useful for power savings. By conducting a series of systematic studies, combining strain engineering and chemical doping, we show robust signatures of strong electron correlations which classifies these primarily as Mott-Hubbard type insulators [1-4]. Systematic validations of Mott insulating character in V_2O_3/VO_2 and insights of thermochromicity in VO_2 is presented.

y0032

Synergistic Effect of Electrical Poling on Dielectric Properties of Al-Doped NBT-BT Lead-free Electroceramics

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Effect of electrical poling mainly contributes to getting perfection in electrical polarization, domain engineering, and ordering. Synergetic effect was studied via temperature-dependent dielectric properties of unpoled and poled $(Na_{0.46}Bi_{0.46-x}Al_xBa_{0.08})TiO_3$ (NBAT-BT) for x=0, 0.05, 0.07, and 0.10 electroceramics. This study shows the poled electroceramics have real and accurate dielectric and ferroelectric data. It was observed that the E-field poling process significantly influences the dielectric, ferroelectric, and leakage properties of these electroceramics. Electrical poling neutralizes all defects present in electroceramics and will control the degree of domain wall motion. Therefore, we proposed that before all electrical measurements, poling must carry for all the electroceramics for better and reliable device performance based on NBT-BT electroceramics.

y0034

Microscopic Diffusion in Biomembrane: Effect of Interactions with Drugs

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Lipid bilayer exists in different phases such as crystalline (L_C), gel (L_β), and fluid (L_α). We have investigated diffusion mechanisms in lipid membrane across different phases. The dynamic landscape, found to comprise four distinct motions of the lipids, namely, (i) lateral (ii) internal (iii) bending and (iv) thickness fluctuations, existing over in a wide range of time and length scale. Our studies revealed that dynamics of lipids is strongly correlated with the physical state of the bilayer and presence of drugs significantly alters the dynamical and phase behaviour of the lipid membrane. It is found that interaction between the drugs and biomembrane is a complex interplay between the physical state of the membrane, charge, concentration, molecular architecture of the drugs, and their location within the membrane. Various interesting features such as induced synchronous ordering between polar head groups and tails, new action mechanism of antimicrobial peptides, lateral segregation of lipids, softening of membrane in presence of drugs are observed and will be discussed here.

y0035

Transport Properties and Charge Conduction across Interfaces of Manganite Based Bilayered Thin Films

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In this report, various manganite based bilayered thin films have been investigated for their possible charge transport properties and charge conduction mechanisms. Various external perturbations such as temperature, electric field, voltage, magnetic field, etc have been employed to alter the interface between the thin oxide layer and manganite channel layer thereby to modify the charge conduction across these oxide interfaces in a controlled way. Attempts have been made to understand the presently investigated interfaces through various transport measurements including temperature dependent resistance under different applied electric fields, current–voltage characteristics recorded at different temperatures, electric field dependent isothermal resistance, field effect device characteristics at room temperature and magnetoresistance (MR) measurements across the interfaces understudy.

y0036

Understanding the role of chlorine treatment on some CdTe-based thin layers and interface structures for solar cell applications

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The main motivation behind this research work is to understanding the role of chlorine treatment on some CdTe-based thin layers and interface structures and to develop solar cells having lower thickness of absorber layer to reduce cost and material consumption. The efforts have done to reduce the film thickness almost three times to achieve good efficiency which is found 7.13% and 8.11% for CdTe and CdZnTe solar cells, respectively that is relatively less than higher reported efficiency but the achieved grain size of 2-3μm at reduced thickness which is similar to the grain size of absorber layer of higher efficiency solar cells.

AUTHOR INDEX

PROGRAMME – DAE SSPS 2021

	Day - 1 (Wednesday, 15th December)		Day - 2 (Thursday, 16th December)		Day - 3 (Friday, 17th December)		Day - 4 (Saturday, 18th December)		Day - 5 (Sunday, 19th December)
Session	Registration (08:00 hrs. Onwards)		A 1	A2	A 1	A2	A 1	A 2	A 1
			Superconductivity	Physics Using Neutron and Synchrotron	Experimental Techniques	YAA Presentation	Matter Under Extreme Conditions	Ph. D Thesis Presentation	Energy Materials
9:30-11:00	*Inauguration (09:30 – 10:15)*		S. Patnaik	Debasis Sen	D. Banerjee	*Presentation for Young Achiever Award (YAA)*	Boby Joseph	*Presentation for Best Ph. D Thesis Award*	Balaji P. Mandal
			Girish Sharma	S. K. Rai	K. Prabakar		Ranjan Mittal		Madhu Chennabasappa
	Plenary-1: Amlan J. Pal		*Contributed Oral Presentations*	*Contributed Oral Presentations*	*Contributed Oral Presentations*		K. K. Pandey		Utpal Sarkar
11:00-11:30	***TEA***								
11:30-13:00	*Plenary-2:* Peter Fischer		*Contributed Oral Presentations*	*Contributed Oral Presentations*	*Contributed Oral Presentations*	*Presentation for YAA*	*Contributed Oral Presentations*	*Presentation for Best Ph. D Thesis Award*	*Poster Presentation*
	Plenary-3: Douglas S. Galvao								
13:00-14:00	***LUNCH***								
14:00-16:00	**THEMATIC SEMINARS**								Concluding Session (14.00-15.00)
	A 1	A2	A1	A2	A 1	A 2	A 1	A 2	
	Quantum Phenomenon	Condensed Matter Theory	Magnetism	Chemical Physics	Strongly Correlated Materials	Glass , Alloy and composite Systems	Nano-Photonics	Surface, Thin Films and Interfaces	
	Pinaki Majumdar	Shobhana Narasimhan	Anamitra Mukherjee	Brendan J. Kennedy	N. S. Vidhyadhiraja	K. R. Pirolkar	Sushil Mujumdar	Sanjay K. Srivastava	
	Bahadur Singh	Brijesh Kumar	Basavaraj Angadi	P. A. Hassan	Subhro Bhattacharjee	Kinshuk Dasgupta	Saikat Ghosh	R. J. Choudhary	
	Anup Kumar Bera	Rajamani Raghunathan	Nirmalaya Ballav	Deepak Chopra	S. Thirupathaiah	S. Abhaya	Jitendra Nath Roy	Suvankar Chakraverty	
	Rajib Batabyal	David J. Singh	*Contributed Oral Presentations*	Ajit K. Mahapatro	Chandrasekhar Murapaka	S. Chatterjee	Mrinal Pal	Satayaprakash Sahoo	
16:00-18:00	*Poster Presentation (including YAA)*		*Poster Presentation (including PhD Thesis)*		*Poster Presentation*		*Poster Presentation*		A1 : Auditorium 1 A2 : Auditorium 2

Venue: DAE Convention Centre, Anushaktinagar, Mumbai