67th DAE
Solid State Physics Symposium

Dec 20 -24,2023

Programme & abstracts

Organized by
Bhabha Atomic Research Centre,
Mumbai

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

Venue
GITAM deemed to be university,
Vishakhapatnam

67th DAE Solid State Physics Symposium

December 20 - 24, 2023

Venue

Gandhi Institute of Technology and Management (GITAM), Visakhapatnam

Organized by Bhabha Atomic Research Centre, Mumbai

Programme and Abstracts

Sponsored by

Board of Research in Nuclear Sciences (BRNS), Department of Atomic Energy (DAE), Government of India

विवेक भसीन
Vivek Bhasin

भारत सरकार
Government of India

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

MESSAGE

It gives me pleasure to note that the 67th DAE Solid State Physics Symposium (DAE-SSPS) is being held at GITAM, Visakhapatnam during December 20 - 24, 2023. The symposium is popularly attended by delegates from all DAE units, universities, national institutes and laboratories working in the areas of condensed matter physics research. Participants look forward to attend this prestigious event, which is organised by BARC annually in various parts of the country.

DAE SSPS series have traditionally been providing a unique interactive forum for scientific discussions amongst scientists, engineers and researchers in important and emerging topics of condensed matter physics. The topics include 1D, 2D and quantum materials, glassy phenomena, multiferoics, superconductivity, soft condensed matter physics, single crystals, photo-voltaics, spintronics, low dimensional physics and energy materials. The interest and popularity of this symposium amongst the condensed matter physics community is well indicated by the large number of nearly 850 manuscripts received this year under the various categories. It is nice to note that the young achiever and PhD thesis awards categories have also received a good response, showing the high value attached to them by the scientific community in the field.

I convey my best wishes for the success of the symposium with intense scientifically scintillating deliberations resulting in new ideas and collaborations.

05.12.2023

(Vivek Bhasin)

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BHABHA ATOMIC RESEARCH CENTRE
भौतिकी वर्ग
PHYSICS GROUP

It is our great pleasure to organize the 67th DAE Solid State Physics Symposium (DAE SSPS 2023). It is indeed a matter of pride and privilege that the Physics Group of Bhabha Atomic Research Centre, Mumbai has been organizing this flagship symposium of the Department of Atomic Energy every year since 1957 in various Indian 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 events are regularly held on various specialized topics covering this subject area.

This year, we were delighted to receive the proposal from Professor Dayananda Siddavattam, the Vice Chancellor of GITAM for organizing the DAE SSPS 2023 at GITAM, Vishakhapatnm. It is also good to note that the DAE is setting up a large BARC-VIZAG campus which includes various high-end R&D programs of the Physics Group of BARC.

In spite of multiple conferences being held in the country, we have received well over 850 manuscripts in SSPS 2023, showing the continued charm of the DAE SSPS amongst the condensed matter research community in the country. The thematic sessions on “Physics at Quantum Scale and Photonics” and “Quantum Material” are included in the deliberations this time, to commemorate the Nobel Prize 2023 in Physics and Chemistry for attosecond physics and quantum dots. The symposium also includes 1D and 2D materials taking note of the current trends in global research interests towards quantum science and quantum computation.

My colleagues, Dr. L M Pant and his team from Physics Group, BARC along with Prof. G. Ravikumar and his team at GITAM, Vishakhapatnam have put in intense and admirable efforts for organising this symposium.

I extend my warm greetings to all the distinguished delegates and participants. I look forward to fruitful and exciting scientific deliberations in the DAE SSPS 2023.

(S. M. Yusuf)

GITAM
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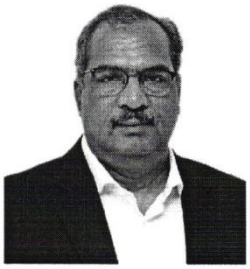
(Deemed to be University)
Visakhapatnam | Hyderabad | Bengaluru

Prof. Dayananda Siddavattam
Vice-Chancellor



Prof. Dayananda Siddavattam
Vice-Chancellor

Message

It is with immense pleasure that I extend a warm welcome to all the delegates, invitees, and participants to the 67th DAE Solid State Physics Symposium 2023, a testament to the Department of Physics, GITAM School of Science's dedication to fostering scientific excellence. I express our profound gratitude to the Department of Atomic Energy for entrusting us with the privilege of hosting this prestigious symposium for the first time at GITAM University. The convening of this esteemed gathering of scientists and researchers from across India and abroad is a matter of immense pride for our institution, and we are honored to provide a platform for insightful discussions and collaborations in the fascinating realm of Condensed Matter Physics. I am confident that this symposium will serve as a catalyst for propelling groundbreaking advancements in Condensed Matter research within the country.

GITAM University is embarking on a transformative journey, evolving from a primarily teaching-oriented institution to one that places paramount importance on research, innovation, and entrepreneurship. As a testament to this commitment, GITAM has forged collaborative partnerships with research groups at BARC Facilities Visakhapatnam, exploring cutting-edge avenues in thin films, and materials processing using ultra-high pulsed magnetic fields and pulsed currents. Our faculty members maintain active collaborations for leveraging the neutron and synchrotron facilities of DAE, underscoring our unwavering dedication to pushing the boundaries of scientific discovery. We anticipate that this event will serve as a catalyst for fostering even deeper collaborations between our faculty and the esteemed condensed matter physics community in India.

We are confident that this symposium will serve as a fertile ground for intellectual exchange and the forging of new scientific partnerships. We extend our heartfelt gratitude to BARC and DAE for their unwavering support in making this event a reality.

(DAYANANDA SIDDAVATTAM)

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अध्यक्ष, तकनिकी भौतिकी प्रभाग
Outstanding Scientist
Head, Technical Physics Division

सत्यमेव जयते

भारत सरकार
Government of India

Message

It is a great privilege to be given the responsibility of organizing the prestigious event of DAE Solid State Physics Symposium. It is also a matter of pride that Gandhi Institute of Technology and Management (GITAM), Visakhapatnam, is hosting the 67th of DAE SSPS series, during December 20-24, 2023.

DAE SSPS has a reputation for covering all the important and emerging areas in condensed matter physics. This year, the categories of materials include Soft Condensed Matter including Polymer & Biological Systems, Nano Materials, Semiconductors, Energy Materials, 1-D and 2-D Materials &Thin films, Single crystals and Glasses with themes on Magnetism & Superconductivity, Spintronics, Transport properties and Phase transitions.

We have received nearly 850 papers this time, out of which 730 manuscripts were accepted for the presentation after they were reviewed by nearly 350 referees form all over the country. The technical sessions include plenary talks, invited talks, contributory oral & poster presentations, PhD thesis and presentations by Young Achiever Award nominees.

I must acknowledge the efforts of the scientific secretaries, Dr. Mohit Tyagi and Dr. Jitendra Bahadur in formulating an excellent program by their dedication and hard work. The sincere efforts of Prof. G. Ravikumar, Local Convener for the excellent synergy in organizing an event of this scale are also worthy of appreciation.

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

11th December 2023

Dr. L. M. Pant
Convener, DAE-SSPS-2023

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भा प अ कें
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SUBJECT CATEGORIES

A. Phase transitions and dynamics

B. Soft matter including polymer and biological systems

C. Nano-materials

D. Experimental techniques and devices

E. Single crystals, glasses and amorphous systems

F. Surfaces, interfaces, and thin films

G. Computational methods, and electronic structures

H. Dielectric, ferroelectric and piezoelectric

I. Transport properties

J. Semiconductor and spintronics

K. Magnetism and superconductivity

L. Energy materials

M. 1-D, 2-D and quantum material

AWARD CATEGORIES

TH: Ph. D thesis Award

YAA: Young Achiever Award Best Poster Award

Program Overview

Day 1: Wednesday, December 20, 2023

(Venue: Yellapragada Subbarao Auditorium)

08:30-09:30	**Registration**
09:30-10:30	**Inaugural Function**
10:30-11:10	**PL-01:** Deepak Dhar, IISER Pune *A new approach to the equation of state for hard spheres* **Session Chair:** D. D. Sharma, IISC Bangalore
11:10-11:40	**High Tea**
11:40-12:20 **12:20-13:00**	**PL-02:**D. D. Sarma, IISC Bangalore *Dynamics of Organic moieties in Hybrid Halide Perovskites and why we should care about it* **PL-03:** Hari Srikanth, University of South Florida, USA *Thermomagnetic spin transport in rare-earth (RE) iron garnet heterostructures* **Session Chair:** Ashok K. Ganguli, IISER Berhampur
13:00-13:15	**Group Photo**
13:15-14:30	**Lunch**
14:30-16:30	**PL-04:** Ashok K. Ganguli, IISER Berhampur *Superconductivity and magnetism in metal chalcogenides* **PL-05:** S. Sastry, JNCSAR, Bengaluru *Plasticity and Yielding in Amorphous Solids* **PL-06:**S. M Sharma, BARC, Mumbai *TBA* **Session Chair:** Deepak Dhar, IISER Pune
16:30-18:30	**Tea and Poster Presentation**
	a0001 to a0008, b0001 to b0007, c0001 to c0023, d0001to d0012, e0001 to e0008, f0001 to f0014, g0001 to g0012, h0001 to h0011, i0001 to i0007, j0001 to j0006, k0001 to k0016, l0001 to l0019, m0001 to m0007, y0001 to y0023
18:30-19:30	**Evening Talk- K S Krishna, Dean, School of Science, GITAM** *Magnetic Field Signatures: an approach for dating the ocean floor* **Session Chair:** G. Amarendra, NFC Hyderabad

Day 2: Thursday, December 21, 2023

(Auditorium 1- Shivaji Auditorium

Auditorium 2- Mother Teresa Auditorium)

09:30-11:00	**Session 1: Soft matter and Biophysics** ***(Venue: Auditorium 1)*** **Session Chair:** S. Sastry, JNCSAR, Bengaluru
	IT-1: B. V. R. Tata, GITAM University, Vizag *Soft and Responsive Hairy Balls: Unusual Dynamics and Yielding of Dense Colloidal Microgel Glasses* **IT-2:** Tapomoy Bhattacharjee, NCBS, Bengaluru *Single-cell morphology dictates bacterial population growth under 3D confinement* **IT-3:** Basavaraj M. Gurappa, IITM, Chennai *Association between like charged surfactants and particles in solution*
09:30-11:00	**Session 2: Magnetism** ***(Venue: Auditorium 2)*** **Session Chair:** S. M. Yusuf, BARC, Mumbai
	IT-4: Anushree Roy, IIT, Kharagpur *Raman Fingerprints of Magnetoelastic Coupling in Complex Oxide Systems* **IT-5:** Saurabh Giri, IACS, Jadavpur *Magnetoelectric coupling without long-range magnetic order in multiferroics* **Contributed Oral Presentations** k0019, k0021
11:00-11:30	**Tea Break**
11:30-13:00	**Contributed Oral Presentations** ***(Venue: Auditorium 1)*** **Session Chair:** Chaitanya Varma, GITAM
	a0011, a0016, b0019, b0031, c0002, c0020
11:30-13:00	**Contributed Oral Presentations** ***(Venue: Auditorium 2)*** **Session Chair:** Vaishali Bambole, Univ. of Mumbai
	c0021, c0027, c0119, d0042, e0006, f0005
13:00-14:00	**Lunch Break**
14:00-16:00	**Session 3: Strongly correlated system and Superconductivity** ***(Venue: Auditorium 1)*** **Session Chair:** Anil K. Bhatnagar, Univ. Hyderabad

	IT-6: Pratap Raychaudhuri, TIFR, Mumbai *Visualising vortex liquid states in superconducting thin films* **IT-7:** Ajay K. Mishra, BARC, Mumbai *Quest for Room Temperature Superconductivity in Hydrogen Rich Materials* **Contributed Oral Presentations** g0022, m0012
14:00-16:00	**Session 4: Novel materials for energy conversion & storage** ***(Venue: Auditorium 2)*** **Session Chair:** B. V. R. Tata, GITAM University, Vizag
	IT-8: Vivek Polshettiwar, TIFR, Mumbai *Unlocking the Potential of Plasmonic Hot Electrons: Black NanoGold for Sustainable Energy and Carbon Management* **IT- 9:** R. S. Dhaka, IIT Delhi *Development of cost-effective energy storage devices* **IT-10:** Arup K. Rath, NCL, Pune *Near-infrared quantum dots for next-generation solar cells* **Contributed Oral Presentations** d0020**,** j0006
16:00-18:00	**Tea and Poster Presentation *(Venue: Auditorium 1)***
	a0009 to a0016, b0008 to b0014, c0024 to c0047, d0013 to d002, e0009 to e0014, f0015 to f0030, g0013 to g0020, h0012 to h0016, i0008 to i0011, j0007 to j0009, k0017 to k0032, l0020 to l0038, m0008 to m0013, t0001 to t0043
18:00-19:30	**Cultural Programs**

Day 3: Friday, December 22, 2023

09:30-11:00	**Session 5: Novel experimental techniques for condensed matter** ***(Venue: Auditorium 1)*** **Session Chair:** Sugata Ray, IACS, Jadavpur
	IT-11: Sandip Ghosh, TIFR, Mumbai *Modulated Optical Spectroscopy For Studying Electronic Bandstructure Of Semiconductors* **IT-12:** Harish N S Krishnamoorthy, TIFR, Hyderabad *Nanophotonics with Topological Insulator Materials*

	IT-13: S.K. Sharma, BARC, Mumbai *Positronium: A Versatile Probe for Material Characterization and Advanced Physics Experiments*
09:30-11:00	**Young Achiever Award Presentations** ***(Venue: Auditorium 2)*** **Session Chair:** K. Maiti, TIFR, Mumbai
11:00-11:30	**Tea Break**
11:30-13:00	**Contributed Oral Presentations** ***(Venue: Auditorium1)*** f0063, g0016, h0021, j0025, l0022, l0099 **Session Chair:** Kavita Chandu, GITAM
11:30-13:00	**Young Achiever Award Presentations** ***(Venue: Auditorium 2)***
13:00-14:00	**Lunch Break**
14:00-16:00	**Session 6: Multifunctional materials** ***(Venue: Auditorium 1)*** **Session Chair:** Mala N. Rao, BARC Mumbai
	IT-14: Sugata Ray, IACS, Jadavpur *Planning new ways of introducing ferroelectricity along with magnetism* **IT-15:** Tathamay Basu, Rajiv Gandhi Institute of Petroleum Technology, India *Spin-driven ferroelectricity from 4d-4f cross-coupling in the strongly correlated system, Ba3HoRu2O9* **IT-16:** D. Bhattacharyya, BARC, Mumbai *Probing electronic & local structures of electrode materials of Li ion batteries by Operando XAS measurements using Indus-2 synchrotron radiation source* **Contributed Oral Presentations** h0050, i0015
14:00-16:00	**Session 7: Topological materials** ***(Venue: Auditorium 2)*** **Session Chair:** K. V. Ramesh, GITAM
	IT-17: Nitesh Kumar, SNBNCBS, Kolkata *From large to zero anomalous Hall effect in the ferromagnetic state of a layered magnet*

	IT-18: Surajit Saha, IISER, Bhopal *TBA* **IT-19:**Srijani Mallick, CNRS, France *Spin-Orbitronics and Superconductivity with KTaO3 based two-dimensional Electron Gases* **Contributed Oral Presentations** e0039, l0057
16:00-18:00	**Tea and Poster Presentations *(Venue: Auditorium 1)***
	a0017 to a0023, b0015 to b0020, c0048 to c0078, d0022 to d0031, e0015 to e0025, f0031 to f0057, g0021 to g0033, h0017 to h0028, i0012 to i0022, j0010 to j0016, k0033 to k0053, l0039 to l0061, m0014 to m0022

Day 4: Saturday, December 23, 2023

	Session 8: Surface and Interface Physics ***(Venue: Auditorium 1)*** **Session Chair:** Bharat Jalan, University of Minnesota, USA
09:30-11:00	**IT-20:** Krishnakumar Menon, SINP, Kolkata *Spectromicroscopy of Surfaces and Interfaces* **IT-21:** Indranil Sarkar, INST, Mohali *Interface electronic structure driven control of spin pumping in ferromagnet/non-magnetic heterostructures* **IT-22:** Mayank Srivastava, IISC, Bangalore *Two-Dimensional Materials: Technological Challenges Ahead*
09:30-11:00	**Thesis Presentation** ***(Venue: Auditorium 2)***
11:00-11:30	**Tea Break**
11:30-13:00	**Session 9: Single crystals and semiconductors** ***(Venue: Auditorium 1)*** **Session Chair:** Anil K Chauhan, BARC Mumbai
	IT-23: Bharat Jalan, University of Minnesota, USA *Modern Approaches in Epitaxy of Quantum Materials* **IT-24:** R. Radhakrishnan Sumathi, Leibniz-Institutfür Kristallzüchtung, Germany *Crystalline materials: Embracing the redefinition of physical unit "kg-mass"*

	IT-25: Swastik Mondal, CSIR-Central Glass and Ceramic Research Institute *High-resolution surface charge density from conventional bulk single-crystal X-ray diffraction data*
11:30-13:00	**Thesis Presentation** ***(Venue: Auditorium 2)*** **Session Chair:** Dr. A.Thamizhavel, TIFR Mumbai
13:00-14:00	**Lunch Break**
14:00-16:00	**Session 10: Physics at quantum scale and photonics** ***(Venue: Auditorium 1)*** **Session Chair:** Krishnakumar Menon, SINP, Kolkata
	IT-26: Sushil Majumdar, TIFR, Mumbai *Machine Learning Approach towards Estimation of Complex Fields From Far-field Measurements* **IT-27:**Gopal Dixit, IITB, Mumbai *Attosecond Physics: Let there be light and electron* **IT-28:**Himanshu Singhal, RRCAT, Indore *Generation of attosecond pulses and their characterization using FROG-CRAB technique* **Contributed Oral Presentations** f0006, m0013
14:00-16:00	**Session 11: Advanced materials for energy and environment** ***(Venue: Auditorium 2)*** **Session Chair:** R. Mittal, *BARC Mumbai*
	IT-29: Samaresh Das, IIT Delhi *Infrared and THz Detectors based on Layered Materials* **IT-30:** Mayank K Gupta, BARC, Mumbai *Fast Ion Dynamics and Phonons in solid Ionic conductors: A Perspective from Neutron Scattering Experiments and Simulations* **IT-31**: Manju Unnikrishnan, CSIR-IMMT, Bhubaneswar *Designing Transparent Conducting Materials for Smart Devices through Band gap Engineering* **IT-32:** N.S. Ramgir, BARC, Mumbai *ZnO: An Efficient Chemiresistive Gas Sensing Material of the Past, Present And Future*

16:00-18:00	**Tea and Poster Presentation *(Venue: Auditorium 1)***
	a0024 to a0031, b0021 to b0026, c0079 to c0113, d0032 to d0037, e0026 to e0038, f0058 to f0071, g0034 to g0054, h0029 to h0046, i0023 to i0029, j0017 to j0024, k0054 to k0069, l0062 to l0088, m0023 to m0029
18:00-19:30	**Interaction with Sponsors**

Day 5: Sunday, December 24,2023

09:30-11:00	**Session 12: Spin liquids and low dimensional magnetism** ***(Venue: Auditorium 1)*** **Session Chair:** V. K. Aswal, *BARC Mumbai*
	IT-33: Narayan Mohanta, IIT Roorkee *Magnetic skyrmions and resonant spin excitation in two dimensions* **IT-34:** A. K. Bera, BARC, Mumbai *Emergent many-body composite excitations and novel quasi particles of 1D quantum spin-1/2 trimer-chains* **Contributed Oral Presentations** k0024, l0025
11:00-11:30	**Tea Break**
11:30-13:15	**Poster Presentations *(Venue: Auditorium 1)***
	a0032 to a0036, b0027 to b0032, c0114 to c0142, d0038 to d0045, e0039 to e0048, f0072 to f0082, g0055 to g0069, h0047 to h0058, i0030 to i0036, j0025 to j0029, k0070 to k0079, l00089 to l0106, m0030 to m0035
13:15-14:00	**Lunch Break**
14:00-15:30	**Award Presentations and Concluding Session** ***(Venue: Auditorium 1)***

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ABSTRACTS

Plenary Talks

PL-01

A new approach to the equation of state for hard spheres

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Finding the equation of state for hard spheres is a classical problem in equilibrium statistical physics. The exact solution is known only in one dimension. For two and three dimensions, over one hundred different approximate equations of state have been proposed in the last one hundred years! In higher dimensions, virial coefficients have been determined numerically for over 70 orders, in dimensions up to 100. However, all these suffer from the problem that they typically only work in only one of the low- or high- density regimes, they do not correctly predict the fluid-crystalline state transition, and they do not have the correct expected singularity structure of pressure P(z) as a function of the activity z. I will discuss an approach, based on the structure of Yang-Lee density of zeroes in the complex activity plane, that can overcome these problems, and can even address the equation for the metastable glassy phase.

PL-02

Dynamics of Organic moieties in Hybrid Halide Perovskites and why we should care about it

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The last decade has seen the most spectacular rise of the halide perovskites with the general formula of ABX_3, where most commonly A = $(CH_3NH_3)^+$ (MA), $(CH(NH_2)_2)^+$ (FA) or Cs^+, B = Pb^{2+} or Sn^{2+}, and X = I^-, Br^- or Cl^- for their superlative photovoltaic and light emissive properties. $MAPbI_3$ is the most investigated among the pure systems. However, rapid degradation of its performance has been a vexing issue, ameliorated by *A*-site cationic substitutions, such as in $MA_{1-y}FA_yPbX_3$. However, the microscopic changes brought about by such substitutions are poorly understood. In this talk, I shall present our efforts at understanding the dynamical aspects of the organic units and their impacts on physical properties by first investigating the pure end-members, $APbX_3$ (A = MA, FA, or Cs and X = I, Br, or Cl) and then by contrasting these with the *A*-site cation substituted systems, $A_{1-y}B_yPbX_3$ to unravel several interesting changes.

This work is a result of collaborations[1-9] with P Acharyya, B Bhattacharyya, K Biswas, M Bokdam, C De, J. P. Embs, C Franchini, S Ghara, A Ghosh, N Kaur Gill, TN Guru Row, A Hossain, BP Kore, G Kresse, A Kumar, J Lahnsteiner, P Mahale, A Mohanty, S Mukherjee, R. Mukhopadhyay, S Pal, A Pandey, D Pariari, MS Pavan, S Picozzi, T Sander, S Sett, Sharada G, V. K. Sharma, A Sinha, A Stroppa, A Sundaresan, D Swain, M. Tyagi, and U Waghmare.

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PL-03

Thermomagnetic spin transport in rare-earth (RE) iron garnet heterostructures

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Spin-heat coupling and thermo-spin transport are topical areas of interest for the spintronics community. The origin of longitudinal Spin Seebeck effect (LSSE) and its relationship with magnetic anisotropy as well as magnon propagation across magnetic insulator/heavy metal interfaces have remained challenging issues. We have pioneered the technique of RF transverse susceptibility to probe the effective magnetic anisotropy in magnetic materials and heterostructures. Combining the RF transverse susceptibility with LSSE measurements, we have shown correlation between bulk and surface anisotropy with the field and temperature dependence of LSSE in YIG/Pt heterostructures and other compensated ferrimagnets [1]. Recently, our group has shown, for the first time, a scaling of LSSE in GdIG/Pt bilayers with different thickness and on different substrates across the compensation temperature [2]. Our ongoing work on TmIG/Pt heterostructures with varying film thickness reveals the clear role of anisotropy and Gilbert damping on the LSSE [3]. From RF susceptibility, LSSE and broadband FMR experiments, quantitative analysis of the magnon propagation length and its correlation with magnetic anisotropy and Gilbert

damping has been demonstrated. Overall, this talk would present new results in the thermal spin transport of garnet heterostructures which are of fundamental importance in spintronics.

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2. "Scaling of the thermally induced sign inversion of longitudinal spin Seebeck effect in a compensated ferrimagnet: role of magnetic anisotropy" -A. Chanda, C. Holzmann, N. Schulz, J. Seyd, M. Albrecht, M.H. Phan and H. Srikanth, **Advanced Functional Materials 32,** 2109170 (2022)
3. "Controlling magnonic spin current through magnetic anisotropy and Gilbert damping" -A. Chanda, C. Holzmann, N. Schulz, A. Ullrich, M. Albrecht, M.J. Gross, C.A. Ross, D.A. Arena, M.H. Phan and H. Srikanth, arXiv preprint arXiv:2308.07236 (2023)

PL-04

Superconductivity and magnetism in metal chalcogenides

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Materials with frustrated magnetism have been studied to understand the origin of frustration among interacting spins. Presence of different interacting magnetic ions in the lattice, possible charge ordering at certain temperatures leads to ferromagnetic (FM) and antiferromagnetic (AFM) interactions in competitive magnetic phases. Apart from the above, the noncentrosymmetric (NCS) nature of crystal lattices also may play a role to generate frustrated magnetic systems [1, 2]. Th_3P_4-type of rare-earth chalcogenides (Ce_3Se_4 and Nd_3Se_4) having noncentrosymmetry have been investigated by us. Ce_3Se_4 has been observed to be ferromagnetic below ~6.5 K. Nd_3Se_4 has been found to be ferromagnetic with T_C= 53 K. Nd_3Se_4 shows metallic behaviour strong interaction among magnetic moments and conducting electrons. From detailed magnetization entropy study and AC susceptibility study, we have shown competing magnetic interactions present in the both these compounds[3]. We also discuss superconducting properties in the La-analog , La_3Se_4 [4].

We have synthesized highly pure phases in polycrystalline $A_2B_3Te_5$ [5, 6] structures by solid state reaction technique and studied its magnetotransport properties. We have studied magnetoconductivity and shown the existence of significant electron-phonon interaction involved in this bulk material.

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PL-05

Plasticity and Yielding in Amorphous Solids

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The mechanical response of a wide range of amorphous solids is of interest in diverse contexts, from molecular glasses, a variety of soft materials such as polymeric glasses, colloids, to granular matter including in geological contexts. Amorphous solids exhibit microscopic aspects of plastic deformation that are distinct from crystalline solids. The nature of such plasticity and the eventual yielding behavior have been investigated extensively in recent years through computer simulations and statistical mechanical approaches, which will be briefly reviewed. In particular, yielding under cyclic shear deformation has been characterized in detail in computer simulations as a sharp, discontinuous transition, which further exhibits striking dependence on the degree of annealing of the amorphous solids subjected to shear. Several of the interesting features observed in simulations are well captured by theoretical models and simulation of elasto-plastic models, while several basic questions remain. The successes and limitations of our present understanding will be summarized.

PL-06
S. M. Sharma, BARC, Mumbai
TBA

ET-01
TBA

ET-02
Magnetic Field Signatures: an approach for dating the ocean floor
K S Krishna, Dean, School of Science, GITAM

Invited Talks

IT-01

Soft and Responsive Hairy Balls: Unusual Dynamics and Yielding of Dense Colloidal Microgel Glasses

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Poly (N-isopropylacrylamide) (PNIPAM) microgel particles are soft spheres with a core-shell structure having a dense polymer core and thin shell consisting of less cross-linked polymers and dangling polymer chains (hairs). Dense suspensions of these hairy soft-spheres exhibit structural ordering similar to that observed in atomic systems. Ordered structures of these microgel suspensions exhibit series of phase transitions with increase in temperature and osmotic pressure. In this talk I will present results obtained by performing investigations using static and dynamic light scattering, UV-Visible spectroscopy and rheology results on ordered (crystalline) and disordered (glassy) structures of thermo-responsive and pH responsive microgel suspensions with volume fractions, $\phi < 0.74$ and under over packed ($\phi > 0.74$) conditions. Under over packed conditions we show that these soft spheres undergo deswelling and exhibit unusual dynamics at short times. The talk presents two surprising results on PNIPAM microgel suspensions under over packed conditions: (i) observation of stable FCC-HCP coexistence in microgel crystals and (ii) two step yielding in microgel glasses. The entanglement of hairs between neighboring soft-spheres under over packed conditions are shown to be responsible for the above mentioned results. To provide an unambiguous evidence in favor of existence of entanglements, we prepared microgel particle without hairs, i.e. particles having only homogeneous polymer core. Non-linear rheological studies and dynamic light scattering measurements on a dense glassy sample indeed showed only single step yielding and absence of sub-diffusive behavior at short times, respectively. These observations constitute evidence in favor of presence of entanglements between hairs and understanding for the unusual behavior of dense microgel crystals and glasses of core-shell structured stimuli responsive microgel particles. Functionality of dangling chains in stabilizing HCP structure over FCC will also be discussed.

IT-02

Single-cell morphology dictates bacterial population growth under 3D confinement

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Can physical properties of the microenvironment act as selection pressures at the population-level? Our current understanding of factors that exert such effect on population growth dynamics implicates genetic mutations and chemical cues, based on experimental assays performed using homogeneous liquid or 2D cultures. However, in their natural niche, bacteria inhabit complex and disordered 3D microenvironments with diverse mechanical properties. Here, to test if the physical microenvironment can selectively favor the collective growth of certain microbial strains under 3D confinement, we design transparent porous 3D growth media that match the viscoelastic properties of natural microbial habitats. Combining optical density-based growth measurements, 3D confocal microscopy, and agent-based simulations, we find that the shape anisotropy of high-aspect-ratio bacteria provides them with a selective advantage to grow more efficiently under increased 3D confinement as opposed to spherical bacteria. More precisely, under 3D confinement, high aspect ratio bacteria produce elongated colonies with larger surface areas allowing them to access nutrients more effectively. Our work provides an example of how the alteration in the physical of the microenvironment can dictate the microbiome composition in 3D disordered materials. This will help in understanding and modeling population dynamics within microbial communities inhabiting diverse biological niches using elementary physical principles.

IT-03

Association between like charged surfactants and particles in solution

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Addition of particles to surfactants is a simple and effective strategy to tailor the structure and flow properties of single or multi-component soft-material systems. Surfactants are typically added to colloidal dispersions to engineer their stability and also during the production of emulsions/foams. Many formulations in diverse industrial sectors essentially are binary particle-surfactant mixtures. Therefore, the investigation of particle-surfactant association in solution is crucial to technological developments in various disciplines. In this study, we address fundamental questions concerning association of similarly and oppositely charged surfactant-particle binary mixture in dilute as well as concentrated regimes. We show that the adsorption of surfactant molecules on the particle surface provides an excellent opportunity to impart exceptional rheological response of surfactant solutions. The role of size, shape, surface charge, and surface chemistry of particle on the rheology and micro-structure will be discussed.

IT-04

Raman Fingerprints of Magnetoelastic Coupling in Complex Oxide Systems

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Lattice degrees of freedom play a crucial role in determining various magnetic phenomena, like spin compensation, multiferroicity, domain wall inversion, or multiple magnetic phase transitions in complex oxide systems. In this talk, I will mainly focus on the coupling of electronic spin and density of states with phonon across two magnetic sublattices in Cr-doped lithium ferrite spinels. The involvement of phonon in governing the magnetic compensation phenomenon in these compounds via the cross-talk between two sublattices will be discussed [1]. The co-existence of spin-phonon and electron-phonon coupling opens a new horizon beyond spin electronics, due to the availability of phonon as a third degree of freedom, for various technological applications of this battery material. To the end, a more generalized view on the importance of magnetoelastic coupling in magnetic materials will be presented through a discussion on spin-phonon coupling in determining multiple magnetic and electrical phases in manganites [2].

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IT-05

Magnetoelectric coupling without long-range magnetic order in multiferroics

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Advancing multiferroic materials to exhibit substantial magnetoelectric coupling at room temperature is a primary objective in the field of multiferroics. Particular attention has been devoted to enhancing magnetoelectric coupling. Conventionally, magnetoelectric coupling has been achieved in multiferroics below the threshold of long-range magnetic order. In this context, we will explore a few exceptions where magnetoelectric coupling has been observed, even in the absence of long-range magnetic order. We will examine three distinct scenarios: the Kagome staircase lattice [1], the layered honeycomb lattice structure [2], and the disordered double perovskite structure [3].

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IT-06

Visualising vortex liquid states in superconducting thin films

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When a magnetic field is applied in a Type II superconductor, the magnetic flux disperses inside the superconductor forming quantized flux tubes (each carrying a magnetic flux), that arrange themselves forming a period structure, called the Abrikosov vortex lattice. While in many ways the vortex lattice behaves like a soft crystalline solid, melting of this solid into vortex liquid state is rarely observed in conventional 3-dimensional superconductors. On the other hand, over the past few years, work carried out in our group showed that vortex liquid states can be realised in superconducting thin films, where the 2-dimensional vortex lattice is much more susceptible to thermal fluctuations. In this talk, I will describe how the melting of a 2-dimensional vortex solid can be directly visualised using a low-temperature scanning tunnelling microscope (STM) and elucidate the structure and dynamics of the 2-dimensional vortex liquid.

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IT-07

Quest for Room Temperature Superconductivity in Hydrogen Rich Materials

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Superconductivity is an enigmatic electronic phenomenon in condensed matter, a marvellous exhibition of cooperative nature of conduction electrons in the form of a condensate of cooper pairs. Although this phenomenon has been observed at low temperatures, e.g. T_C for mercury Hg is 4.2 K, the quest for room temperature superconductor has been a holy grail for the researchers. N. W. Ashcroft predicted the compressed hydrogen to be metallic and room temperature superconductor beyond ~ 75 GPa [1]. However, this goal is still elusive. Later, the idea of precompressed hydrogen in a metallic lattice was floated leading to the search for hydrogen rich materials [2]. There have been several predictions of hydrogen rich hydride materials with high T_C values [3]. The superconducting properties of these hydride materials are mainly based on the electron-phonon interaction (conventional BCS type). In this talk we will present an overview of the recent developments in the field [4] along with our own discovery of superconducting lanthanum superhydride (LaH_{10}) starting from prediction [5] to its synthesis at extreme conditions [6,7] and experimental observation of high T_C ~ 260 K [8].

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IT-08

Unlocking the Potential of Plasmonic Hot Electrons: Black NanoGold for Sustainable Energy and Carbon Management

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We are creating new nanocatalysts by precise morphological control of nanomaterials like dendritic fibrous nanosilica (DFNS)[1] to advance catalysis and solar energy harvesting. DFNS was then used to design some unique catalysts, such as Black Gold[2], Defective Catalysts[3,4], Solid Acids Nanosponges[5], Lithium Silicate Nanosheets[6], and Plasmonic Nanocatalysts.[7,8]

In this talk, I will discuss one of our recent works on solar energy harvesting and CO_2 utilization, using the concept of *"Hot Electrons in Plasmonic".* We transformed yellow gold into "*Plasmonic Black Gold*" which harvests board band solar light. We have then synthesized nickel-laden black gold catalysts with a high photocatalytic CO production rate, selectivity and stability.[7] Black Gold-Ni also catalyzes several other reactions, such as H_2 dissociation, C-Cl bond activation, and acetylene semi-hydrogenation, using solar light. The CO_2 hydrogenation reaction mechanism was studied by using (i) finite-difference time-domain simulations, (ii) light-intensity-dependent production rate, (iii) light-intensity-dependent photocatalytic quantum efficiencies, (iv) wavelength-dependent production rate, (v) kinetic isotope effect (KIE), (vi) ultrafast transient absorption spectroscopy, and (vii) in situ diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS).[7,8]

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IT-09

Development of cost-effective energy storage devices

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Abstract:
In recent years, energy storage devices especially rechargeable batteries have become part of our daily life in portable electronic devices like mobiles, laptops as well as being used at large scale in electrical vehicles (EV), etc. As we know, among various types of batteries, the only commercially established and feasible technology is based on Li-ion intercalation, mainly due to the advantage of high energy density, good rate kinetics and light weight. However, the major concern is due to the limited availability and uneven distribution of Li around the world. Among the alternative avenue, the Na-ion batteries are one of the potential candidates particularly for grid level storage due to its low cost and abundance on the globe, and therefore extensive research has been started in this field over past few years [1]. In this direction, it is vital to find suitable electrode materials having high performance. However, there are many challenges mainly due the larger size of the sodium-ion as compared to the Li. Therefore, constant efforts are going on to search new electrode materials (negative as well as positive) for improving the electrochemistry. I will cover basic of battery chemistry and need of development of cost-effective energy storage devices. In the talk, I will discuss some of the results on recently developed cathode and anode materials, and their electrochemical performance to understand the diffusion kinetics, stability, rate capability and coulombic efficiency in sodium ion batteries [2-5].

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IT-10

NEAR-INFRARED QUANTUM DOTS FOR NEXT-GENERATION SOLAR CELLS

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Abstract: The broad tunability of the energy bandgap through size control makes colloidal quantum dots (QDs) promising for the development of photovoltaic devices. Large-size QDs, exhibiting a narrow energy bandgap, are particularly interesting as they can be used to augment perovskite and c-Si solar cells due to their complementary NIR absorption. However, their complex surface chemistry makes them difficult to process for the development of solar cells. Here we report a hybrid passivation strategy for large-size and narrow bandgap QDs to passivate both (111) and (200) facets, respectively, using inorganic lead tri-iodide (PbI_3^-) and organic 3-Chloro-1-propanethiol (CPT). Employing charge balance calculation, we identified the desired narrow bandgap for QDs to complement perovskite and c-Si absorption. The distinct choice of organic ligand CPT enhances the colloidal stability of QDs in the solution phase and improves surface passivation to stop QD fusion in solid films. Photophysical property shows narrower excitonic and emission peaks and a reduction in Stokes shift. Hybrid passivation leads to a 94% increment in the power conversion efficiency of the solar cells and a 74% increase in external quantum efficiency at the excitonic peak.

Keywords**:** solar cells, quantum dot, infrared-bandgap, trap states, polydispersity, surface passivation

Result and discussion

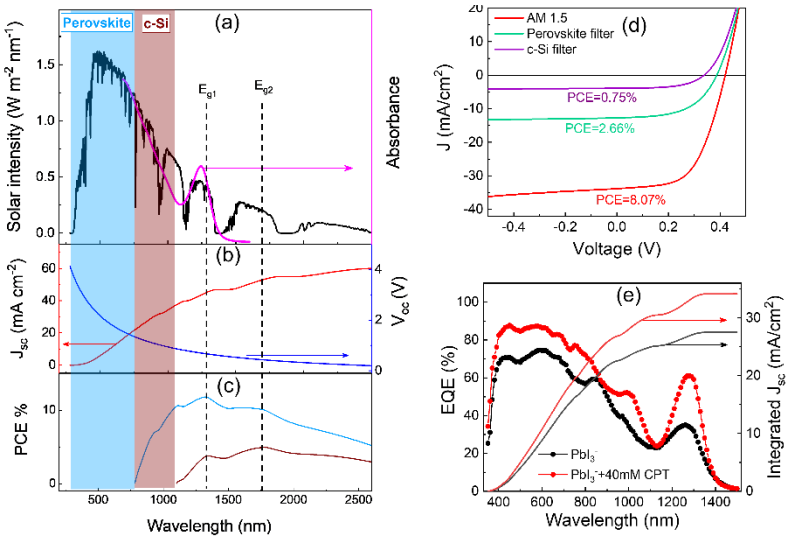

Figure 1. (a) AM1.5G solar spectrum is shown by the black curve. The absorption regions for perovskite and c-Si are marked. The pink curve shows the absorption profile of the PbS QDs used in this study. (b) Evolution of the open-circuit voltage (V_{oc}), and the short circuit current density (J_{sc}) with the bandgap, in single-junction solar cell configuration, using details balanced approach. (c) shows the calculated power conversion efficiency (PCE%) with bandgap (in terms of wavelength) of the bottom QD layer for the photons transmitted by perovskite (light blue line) and c-Si (wine line). E_{g1} and E_{g2} indicate most suitable bandgaps of QDs for multijunction application with perovskite and c-Si. (d) J-V characteristics of the solar cell for optimized ligand condition under full solar illumination, perovskite filter (long pass 780 nm), and c-Si filter(long pass 1100 nm. (e) EQE and calculated J_{sc} of solar cells.

Reference: Chandan Mahajan, Ashish Sharma, Arup K. Rath*; *ACS Appl. Mater. Interfaces, 2020, **12**, 49840-49848.*

IT-11

Modulated Optical Spectroscopy For Studying Electronic Bandstructure Of Semiconductors

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Electronic bandstructures of semiconductors are usually engineered by controlling dimensions, alloying, strain, heterostructure formation etc to suit device applications. Such bandstructure changes are often studied using optical techniques such as photoluminescence and absorption spectroscopy, which have limitations. This talk will introduce modulation spectroscopy and describe different types of modulation techniques involving external electric/magnetic fields, pump laser, strain, temperature etc. with emphasis on photo-reflectance, electro-reflectance spectroscopy. Basic experimental setups and spectral lineshape origins including Franz-Keldysh oscillations will be discussed. The advantage of these techniques will be brought out with examples from studies on group III-V semiconductors and their heterostructures such as quantum wells. Finally I will discuss application of these techniques in our recent studies on 2-dimensional transition metal dichalcogenide semiconductors such as MoS_2 including their monolayers, where they helped provide information on excited states of excitons including new types such as inter-layer excitons, their binding energies and the Lande g-factor.

IT-12

Nanophotonics with Topological Insulator Materials

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Chalcogenide 3D topological insulators belonging to the BSTS [$Bi_xSb_{(2-x)}Te_ySe_{(3-y)}$] family are extremely promising candidates for photonic applications, thanks to their peculiar properties such as bulk plasmonic response in the visible region, high polarizability in the infrared, spin-momentum locking as well as the presence of coupled bulk-surface states. In this talk, I will give a brief overview of these aspects and then focus on our recent work where we show that plasmonic and dielectric regions of the material permittivity gives equivalent performance, thus opening avenues to broadband interband polaritonics with these materials.

IT-13

Positronium: A Versatile Probe for Material Characterization and Advanced Physics Experiments

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Positronium (Ps) is a bound state (binding energy -6.8 eV) of positron and electron, which is formed in low electron density materials. Depending on spin orientation of electron and positron in Ps, two different energy states of Ps viz. singlet (*para*-Ps, *p*-Ps) and triplet (*ortho*-Ps, *o*-Ps) are formed in 1:3 ratios. The intrinsic lifetime of *p*-Ps and *o*-Ps are 0.125 and 142 ns, respectively. Due to long lifetime of *o*-Ps, it interacts with the material during its lifetime, and gets localized in low density regions such as free volume holes in polymers/polymer nanocomposites, pores in porous materials and surface of metal or alloys. Annihilation characteristics of localized *o*-Ps (lifetime, momentum distribution) carry unique information about the materials under investigation. Our recent studies on flexible Zeolitic Imidazolate Frameworks (ZIFs), wherein *o*-Ps has been used to investigate the tuning of pore-structure and framework flexibility under external stimuli will be discussed [1-6]. Through these studies, it has been confirmed that using *o*-Ps probe, pore-structure (pore size, pore-size distribution and pore interconnectivity) of ZIFs can be efficiently determined without any artifact caused by gas-framework interaction induced flexibility of these frameworks, which has hindered the application of gas-adsorption based method for pore-structure determination of these materials. In addition, open volume at pore-site *in-situ* under gas pressure determined using *o*-Ps lifetime spectroscopy is observed to be directly related to the framework flexibility. These studies have established that *o*-Ps lifetime spectroscopy can be used as a routine technique for tuning of pore-structure of ZIFs for their enhanced applications in gas-storage and gas-separation.

In addition, possibilities of Ps as probe for multi-positron physics experiments will also be discussed.

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IT-14

Planning new ways of introducing ferroelectricity along with magnetism

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Abstract : The existing literature on multiferroics categorizes the vast number of potential materials into two classes, such as type-I, where magnetic and ferroelectric orders originate through separate mechanisms, and type-II where ferroelectricity is driven by magnetic order. Type-I multiferroics are further divided into 3 subgroups based on the active mechanism, i.e., lone pair driven, charge order driven, and geometric distortion driven.[1,2] However, search for new multiferroic materials and new mechanisms is ongoing. Interestingly, except for only a few examples, search for such materials had been traditionally focused on oxides, which can offer diverse structures and properties and also are favorite candidates of nature, as suggested by mineralogy. Only recently mixed-anion compounds, in which a metal cation is bonded to more than one anionic ligand, giving rise to variations in charge, ionic radii, electronegativity, and polarizability, are being considered very seriously because they may support various unusual phenomena, nominally inaccessible to their single-anion counterparts. Few recent reviews[3–6] summarize the significant potentials of mixed-anion compounds in the field of catalysis, energy conversion, electronic devices, magnetism, as well as ferroelectricity. Similarly, there are other innovative ways[7-9] by which collective distortion and ferroelectricity can be introduced in systems. In the presentation, I shall try to offer glimpses of such possibilities and also would point out their shortcomings.

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IT-15

Spin-driven ferroelectricity from 4d-4f cross-coupling in the strongly correlated system, $Ba_3HoRu_2O_9$

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I will discuss the spin-driven ferroelectricity and magnetoelectric domain dynamics of the 6H-perovskite multiferroic $Ba_3HoRu_2O_9$ system. The occurrence of spin-driven polarization is rarely observed in a 4*d*/5*d* transition-metal oxides, compared to their 3d-transition-metal oxide counterparts, despite theoretical predictions of the good possibility of multiferroicity in higher *d*-orbital systems. Here we have studied a prototype 4*d*-4*f* compound, $Ba_3HoRu_2O_9$, through time-of-flight neutron diffraction, ac susceptibility, and complex dielectric spectroscopy. We demonstrate that the non-colinear structure involving two different magnetic ions, Ru(4*d*) and Ho(4*f*), breaks the spatial inversion symmetry via inverse Dzyaloshinskii–Moriya (D-M) interaction through strong 4*d*-*4f* magnetic correlation, which results in non-zero polarization. The stronger spin-orbit coupling of 4*d*-orbital might play a major role in creating D-M interaction of non-collinear spins. We have systematically investigated the magnetoelectric domain dynamics in this system, which exhibits intriguing behavior with shorter coherence lengths. Further, we have investigated the effect of external pressure on the magnetic transition. The result reveals an enhancement of ordering temperature by the application of external pressure (~1.6K/GPa). We speculate that external pressure might favor stabilizing the magnetoelectric phase. Our study shows a route to designing magnetoelectric multiferroic compounds containing larger *d*-orbital through strong 4*d*-4*f* cross-coupling.

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IT-16

Probing electronic & local structures of electrode materials of Li ion batteries by *Operando* XAS measurements using Indus-2 synchrotron radiation source

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Over the last few years using the 2.5 GeV Synchrotron Radiation Source (Indus-2) at RRCAT, Indore, India several *operando* X-ray Absorption Spectroscopy (XAS) measurements have been carried out on Li ion batteries for probing changes in electronic and geometric structures of the electrode materials during the electrochemical reactions or charging/discharging cycles of the batteries [1-6]. An electrochemical cell with kapton X-ray windows has been successfully developed in-house for such *operando* XAS and X-ray diffraction measurements on Li-ion batteries using synchrotron source and related facilities have been created at the Scanning EXAFS beamline (BL-09) of Indus-2 for such measurements. *Operando* XAS measurements, on Li-ion batteries with $LiMn_2O_4$ as cathode material during charging and discharging, when Li ions are de-intercalated and intercalated respectively, reveal that electronic and structural changes at the Mn sites of the cathode material during the cyclic processes are not fully reversible. Also, *in-situ* XAS measurements of the layer-structured lithium cobalt nickel manganese oxides ($Li[Ni_xCo_yMn_z]O_2$) or LNMC, which is lately been emerged as one of the highly promising electrode material, have been carried out simultaneously at Co, Ni and Mn edges. Analysis of XAS spectra during charging shows that the major charge compensation at the metal site is achieved by oxidation of Ni^{2+} ions without any change in the oxidation state of Co or Mn ions. This study also shows that local structural changes at Ni sites in the samples with higher Ni concentrations are much less compared to in the samples with lower Ni concentrations during charging/discharging cycles which is a new finding. The structural changes of Fe_3O_4 nanoparticle based electrodes in Li ion battery during charging-discharging cycle have also been investigated using *operando* XAS measurements followed by statistical analysis using Chemometric methods viz., PCA and MCR-ALS. The above measurements clearly identify the four species involved in the whole intercalation-conversion process of Fe_3O_4 electrode of a Li ion battery for the first time in literature and also indicates to the irreversibility of the conversion reaction in subsequent cycles which may be one of the reasons for capacity fading of these electrodes. The talk will also include our recent work on TiO_2 thin film based electrodes prepared using RF magnetron sputtering technique

on polished stainless-steel substrates. Films with amorphous, anatase and rutile phases have been obtained by varying the preparation conditions and batteries have been prepared. During the cycling test, the cell containing rutile phase TiO_2 electrode showed the highest specific capacity of ~1000 $\mu Ahcm^{-2}\mu m^{-1}$ after 700 cycles at a high rate of 100 μAcm^{-2}, which is much higher than any reported value so far. Grazing Incidence X-ray diffraction measurements with a laboratory X-ray source and XAS measurements using synchrotron radiation show a clear signature of rutile to anatase phase transition in the samples during 1st discharge or Li ion insertion process, which is subsequently retained during the 1st charging cycle also. This is further corroborated by the constant voltage plateau observed in the galvanostatic cycle (potential versus capacitance plot) of the Li ion battery also during the 1st discharge cycle. Recently operando XAS measurements have been carried out on Li ion batteries with $MoSe_2$ and hybrid $MoSe_2$@rGO nanocomposites electrodes also, few results of which will also be presented in this talk.

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IT-17

From large to zero anomalous Hall effect in the ferromagnetic state of a layered magnet

Authors: Mahima Singh, Jyotirmoy Sau, Arunanshu Panda, Banik Rai, Manoranjan Kumar, Nitesh Kumar

Abstract: Layered ferromagnets, in particular those with Curie temperature above room temperature are important for spintronic applications. We have investigated the electrical transport properties of single crystals of a room temperature ferromagnet $SmMn_2Ge_2$ with T_C of ~350 K. The case of $SmMn_2Ge_2$ is unique because this enters to an antiferromagnetic state for an intermediate temperature range subsequently going to a ferromagnetic (FM) state at low temperature again. The most important difference between the two ferromagnetic states is the magnetic anisotropy; the easy axis of magnetization for the high temperature FM state is perpendicular to the layers while it is along the layer for the low temperature FM state. We have carried out a detailed study of transport properties of this compound. We discover that a large anomalous Hall effect is entirely of intrinsic origin on the application of magnetic field perpendicular to the layer, and completely extrinsic when applied along the layer. We also support these findings with first principles calculations

IT-18

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TBA

IT-19

Spin-Orbitronics and Superconductivity with $KTaO_3$ based two-dimensional Electron Gases

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The oxide two-dimensional electron gas (2DEG) at the interface between two insulators $SrTiO_3$ (STO) and $LaAlO_3$[1], displays a wide array of functionalities; such as high electronic mobility, low temperature superconductivity,[2] and tunable Rashba spin-orbit coupling (SOC)[3]. Among these, the latter two properties can be utilised to realize devices for the field of topological quantum computing[4] and spin-orbitronics[5]. Along with the experimental observation of record spin Edelstein length in STO based 2DEGs[5], it has also been predicted theoretically that the orbital Edelstein effect exceeds the spin Edelstein effect by more than one order of magnitude in this system[6].

Similar to STO, $KTaO_3$ (KTO) is a quantum paraelectric material where due to the presence of Ta (5d element), the Rashba SOC in this 2DEG is expected to be larger than STO 2DEGs. Although superconductivity in the STO based 2DEGs were observed soon after their realization, the KTO based 2DEGs did not evidence superconductivity until recently when Liu *et al.* reported it with T_C ~2 K (one order of magnitude larger than STO 2DEGs) in (111)-oriented KTO 2DEGs[7]. This observation unlatched a huge platform to examine the superconducting properties of KTO based 2DEGs and nurture them in combination with its inherent high Rashba spin-orbit coupling towards the realization of topological superconducting qubits.

In this work, 2DEGs are generated by the deposition of Al metal on KTO single crystals. Transport and spin-pumping measurements are performed to explore the 2DEG properties and the spin Edelstein effect, respectively[8]. Further, the samples are characterized by angle-resolved photoemission spectroscopy to probe the band structure[9]. In addition, the band resolved spin and orbital Edelstein effects have been computed and we predict that these efficiencies exceed by at least twice than the other oxide 2DEGs[9]. Further, we have used microwave transport to show that KTO (111) 2DEGs exhibit a node-less superconducting order parameter with a gap value significantly larger than expected in a simple BCS weak-coupling limit model. Consistent with the two-dimensional nature of superconductivity, we evidence a well-defined Berezinsky-Kosterlitz-

Thouless type of transition, which was not reported on STO-based interfaces[10]. Finally, we will discuss how our finding offers innovative perspectives for fundamental science as well as for device applications in fields like spin-orbitronics and topological electronics.

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IT-20

Spectromicroscopy of Surfaces and Interfaces

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In this talk, I will discuss different approaches to spectromicroscopic studies at surfaces and interfaces using both electrons and photons as probes. Particularly, the emphasis will be on Low Energy Electron Microscopy (LEEM) and Photoelectron Microscopy (PEEM) methods, with examples from the laboratory as well as synchrotron-based studies. These methods can be used to study different aspects of the surfaces, such as surface structure, morphology, electronic structure and surface magnetism for a wide variety of sample conditions. Interestingly, they can also be employed to unravel the dynamical processes occurring on surfaces and interfaces

IT-21

Interface electronic structure driven control of spin pumping in ferromagnet/non-magnetic heterostructures

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Abstract: Spin pumping is an interesting phenomenon of pure spin current emission into adjacent normal metal in a ferromagnet/normal metal heterostructure. The underlying physics of spin pumping is a consequence of the interaction of magnetic texture dynamics and current. Ferromagnet/heavy metal hetreostructures present quintessential quantum interfaces where spin pumping effect is widely studied both from fundamental perspectives and from spintronic application point of view for spin current generation. This interfacial phenomenon is strongly dependent on the electronic and physical structure of the heterostructure.
In this talk, I will introduce the concept of spin pumping and shall present our recent results of magnetization dynamics and physical and electronic structure evolution across the ferromagnet/heavy metal interfaces. Through this presentation, the correlation between the interface engineering and spin pumping efficiency will be discussed.

IT-22

Two-Dimensional Materials: Technological Challenges Ahead

Mayank Srivastava, IISC, Bangalore

Abstract: This talk will attempt to present the technological and fundamental challenges in pushing 2D technology to the market, where the world stands today, and what gaps are required to be filled. Talking about the gaps, I will particularly touch base on the Metal (3D) to graphene/TMD (2D) contact engineering challenges, which has been considered as one of the most fundamental challenges towards harnessing the full potential of 2-dimensional materials. And, how the fundamental understanding of the contact's quantum chemistry resulted in unique ways to engineer it, resulting in record transistor performance. Besides, I will talk about some of the fundamental process or process-driven reliability challenges that can unintentionally perturb the 2D channel's electrical, optical, and mechanical properties. In the end, I will talk about some of the reliability gaps, which are urgently required to be addressed, and the fundamental understanding we have developed so far.

IT-23

Modern Approaches in Epitaxy of Quantum Materials

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From its beginnings as a successful method for III–V semiconductor growth to today for the growth of many contenders for next-generation electronics, spintronics and quantum devices, molecular beam epitaxy (MBE) has been very successful. However, several challenges exist for metal oxide growth where a metal is hard-to-oxidize and/or difficult to evaporate/sublimate. In this talk, I will review these issues and will present my group's effort to address these challenges using a novel solid-source metal-organic MBE approach. We show, for the first time, controlled synthesis of metal and metal oxides of these "stubborn" elements with the ***same ease and control*** as afforded by III-V MBE. We will present detailed growth study

utilizing chemistry of source materials as a controlling knob to navigate synthesis. With the goal to understand and control electronic ground states in defect-managed complex oxide films and nano-membranes, we will discuss how chemistry of source materials can be used to navigate synthesis on-demand.

IT-24

Crystalline materials: Embracing the redefini on of physical unit "*kg*-mass"

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Abstract: Historically, the kilogram (*kg*) has been defined by a physical alloy ar fact, the Interna onal Prototype of the Kilogram (IPK), a pla num-iridium cylinder stored in France. This has limita ons including the IPK's suscep bility to wear and contamina on leading to uncertain es in measurements. In this talk, an introduc on of redefining the *kg* based on fundamental constants of nature will be given. A'er presen ng an overview of this paradigm shi', this talk presents the efforts and emergence of high purity crystals as crucial materials in advancing the new defini on of the *kg* mass unit. Isotopic silicon-28 (^{28}Si) crystals have been instrumental in this endeavour, offering a more stable, universal mass measurement. The aim is to aid an accurate determina on of the Avogadro constant (N_A) with unprecedented precision. It is well-known that N_A relates the number of atoms or molecules in a substance to its mass. This alterna ve recipe of (re)defining the *kg* involves coun ng the number of atoms in an almost perfectly round, so'ball-sized sphere of ^{28}Si atoms. At IKZBerlin, ^{28}Si single crystals of 4-inch diameter have been grown with very high purity and perfec on. The crystal growth and its processing will be discussed in detail. The significance of ^{28}Si crystalline material in terms of la1ce structure, crystal perfec on, intrinsic proper es in the transforma on of this redefini on, the advantages it offers in terms of excep onal high isotopic purity (reduces uncertain es related to atomic masses), reproducibility and cross-disciplinary compa bility will also be highlighted. Since 2019, ^{28}Si crystals grown at IKZ is serving the purpose of the Avogadro constant determina on and this crystal ball is being currently kept at Sévres near Paris in France.

Reference:

N. V. Abrosimov et al., Metrologia 54 (2017) 599.

IT-25

High-resolution surface charge density from conventional bulk single-crystal X-ray diffraction data

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Abstract: Understanding surface structures in terms of surface charge density distribution has long been a central concern for scientists as the surface structure of materials plays a crucial role in governing their interactions with the external environment. Traditional bulk X-ray diffraction data has historically been considered insufficient for deciphering surface structures, necessitating the use of specialized surface-sensitive techniques. Here, we present a novel approach to extract high-resolution experimental surface charge density distributions from conventional bulk X-ray diffraction data, employing the concept of aspherical charge density models. We show that by excluding the contribution of charge density sources above a surface and accounting for the resulting charge density rearrangements, surface charge density can be obtained from bulk data (Fig. 1). Using accurate multipole models derived from high-resolution single-crystal X-ray diffraction data, we analyzed molecular and extended solids, including α-glycine, α-boron, boron carbide, and calcium mono-silicide. The results highlight significant differences in charge density distributions between bulk and surface, especially in extended solids, emphasizing the importance of considering atom-atom interactions in surface analysis. This method provides a new, accessible avenue for determining surface structures, potentially explaining diverse surface phenomena. The observed differences in charge density distributions between bulk and surface shed light on the underlying mechanisms governing surface-mediated phenomena, offering potential insights for a wide range of applications in materials science and beyond. The method's effectiveness is demonstrated through an analysis of boron carbide, a p-type semiconductor, revealing distinctive electron-deficient centers on specific surfaces explaining its gas-sensing behavior. Overall, this study introduces a powerful technique for extracting high-resolution surface charge density information from conventional bulk X-ray diffraction data.

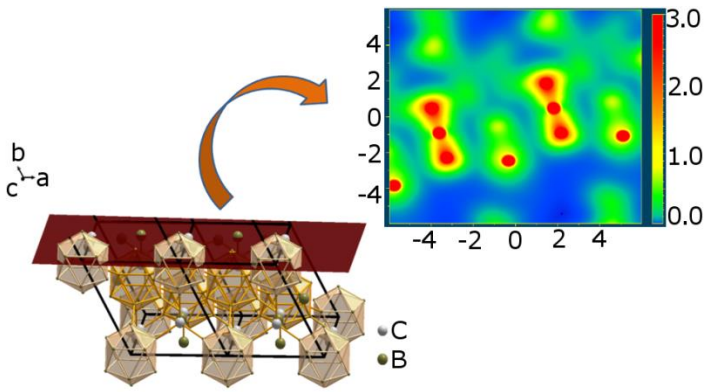

Figure 1: Surface charge density determination from bulk single-crystal X-ray diffraction data.

IT-26

Machine Learning Approach towards Estimation of Complex Fields From Far-field Measurements

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A regular situation encountered in physics research is the comparison of experimental measurements with the existing theory. Towards meaningful comparison, it needs to be ensured that both the experimental observations and theoretical surmises are obtained under identical conditions. In the Optics domain, a situation is often encountered in mesoscopic optical regime, wherein pre-existing theory details the behavior of transport parameters under near-field conditions. On the other hand, optics experiments carry two primary differences, one is that the fields cannot be measured and only intensities are available as measurable quantities, and the second is that near-field measurements are extremely challenging, and most experiments end up making only far-field measurements. In this situation, transport properties are misinterpreted, particularly when one is close to the Anderson localization regime. In the domain of Nanophotonics, since the physical structures are often available to a precise degree, machine learning may allow us to use that information to estimate complex fields from far-field measurements. In this work, we set up neural networks to achieve the same, in a one-dimensional disordered system that was analyzed by a fully connected deep neural network (FCDNN) and a two-dimensional system handled by a convolutional neural network (CNN). We succeed in extracting complex fields in both the cases with an accuracy of more than 95% as quantified from correlation measurements. We elaborate the rectification in inferences obtained from far-field measurements. A well-trained network offered a massive improvement over conventional simulation softwares, thereby justifying the usage of neural networks in Nanophotonics.

IT-27

Attosecond Physics: Let there be light and electron

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Inducing and probing the motion of electrons during numerous physical and chemical processes in real-space and in real-time are of immense importance as it can provide important insights into the mechanisms involved. This year Physics Nobel Prize is awarded to Attosecond Physics and its application to electron motion. In this talk, after discussing the important of attosecond physics, I will showcase few examples of our group where attosecond physics promises to bring technological radical changes, such as light-driven valleytronics and valley transistor, debate about the massless nature of Weyl fermions in Weyl semimetals, attosecond charge migration in molecules to name but a few. The detailed activities of our attosecond group can be seen at https://attosecondindia.com.

IT-28

Generation of attosecond pulses and their characterization using FROG-CRAB technique

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Different fundamental phenomena, such as photo-emission and electron charge migration, occur over attosecond time scale. Generation and measurement of attosecond pulses is essential towards the atom/molecular reaction dynamics as well as for attosecond pulse metrology. One cannot generate attosecond pulses using IR lasers; hence, phase-locked odd harmonics of the laser are generated by its interaction with low-density gas. Overlap of multiple harmonics manifests as an attosecond pulse train (APT) with individual attosecond pulses separated by half of the IR laser cycle. To measure the duration of the APT, we need to measure the relative phase between consecutive harmonics using a cross-correlation method. In this method, the parent fs IR laser and APT is overlapped in a low-density gas sheath. The APT generates photo-electrons corresponding to the photon energy of constituent odd harmonics, and the overlap of the IR pulse generates the sidebands at even harmonic energy. These photo-electrons are detected by a magnetic bottle electron time of flight spectrograph (MBeTOFS). With the change in delay between IR pulses and APT, the photo-electron sidebands' intensity oscillates in time, and the relative position of peaks gives the phase between adjacent harmonics. This method is popularly known as the RABBIT technique. For complete characterization of APT, an iterative algorithm known as FROG-CRAB (frequency-resolved optical gating for complete reconstruction of attosecond bursts) is used.

Here at Laser Plasma Division, RRCAT Indore, we are working towards generation and measurement of attosecond pulses. Interaction of a 6 mJ, 1 kHz, 50 fs Ti:sapphire laser with a gas-filled cell generates its high order odd harmonics. These harmonics are focused in the gas sheath using a toroidal mirror. To detect the photo-electron spectrum and to characterize the attosecond pulse trains, we have developed in-house a high-resolution double solenoid magnetic bottle electron time of flight (MBe-TOF) spectrograph. The MBe-TOf has ~ 60 meV resolution and can easily resolve Ar 3p1/2 and Ar 3p3/2 doublet separated by ~178 meV. The delay between the IR laser and APT is controlled using a closed-loop PZT. The photo-electron spectrum was measured for complete overlap of harmonics and laser pulse. FROG-CRAB algorithm is also developed independently. All the signal processing and data acquisition routines are developed in-house. The CRAB reconstruction gives the duration of the individual as pulses between 300-400 as (FWHM) and duration of APT envelope ~15 fs (FWHM).

IT-29

Infrared and THz Detectors based on Layered Materials

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Infrared and terahertz technology offer significant potential for a wide range of applications, including imaging, communication, material spectroscopy, security, and the biomedical field. These applications demand achieving broad bandwidth, high responsivity, and lower noise-equivalent power (NEP). To address these requirements, there has been a substantial research focus on two-dimensional layered materials such as transition metal chalcogenides (TMC), b-As, and b-P for the development of infrared and terahertz sensors. However, a persistent challenge has been the limited integration capabilities and the development of efficient detectors that can operate at room temperature.

This talk will focus on the design and fabrication of highly efficient detectors utilizing low-dimensional layered transition metal dichalcogenides (TMDs) and black arsenic materials. We will introduce a terahertz detector featuring a type-II topological Dirac semimetal, platinum telluride (PtTe2), tailored for applications in the 0.1-1.5 THz frequency range [1]. Moreover, we will present a self-powered broadband photodetector suitable for near-infrared (IR) and shortwave-infrared (SWIR) applications, based on the MoSe2/GeOI heterostructure. Lastly, we will present a polarization-sensitive SWIR phototransistor established on a black arsenic/GeOI heterojunction [3]. This research offers fresh insights into the use of GeOI as a heterojunction material with layered materials, particularly in the SWIR spectrum, and holds promise for high speed sensing applications.

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IT-30

Fast Ion Dynamics and Phonons in solid Ionic conductors: A Perspective from Neutron Scattering Experiments and Simulations

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Ionic solids, in which mobile ions can diffuse with mobilities comparable to those of liquids, are attracting intense interest for rechargeable batteries and fuel cell applications. Recently, a significant number of Na and Li ionic conductors have been discovered, exhibiting very high ionic conductivity suitable for solid electrolytes. An atomistic investigation of Na diffusion in solid electrolytes and identifying the relevant descriptor would help design better electrolytes. We use a cumulative approach of neutron scattering experiments and theoretical modelling to develop a strategy to understand ion dynamics in these solids[1-10]. We have identified the effect of soft phonons, thermal expansion, and amorphization on ionic diffusion on various Li/Na-based conductors and showed that this could be used as descriptors for designing solid electrolytes. Recently, we demonstrated that the anharmonicity of phonon modes across M-R lines are critical descriptors of Na diffusion in Na-antipervoskites[1]. In quaternary chalcogenides, Na3ZnGaX4 (X= S, and Se), identified that the presence of specific topological cationic sites in the framework structure enables the fast-ionic conduction in Na3PCh[2]. For the first time, our studies on amorphous $Li_2Si_2O_5$ suggest that coupling of the cationic dynamics with the soft dynamics of its neighbouring polyhedral units (SiO_4 /AlO4) enhances the cationic (Li^+) diffusion in amorphous[3]. Our extensive investigation on argyrodites and Na thiophosphate shows the strong influence of low-energy anharmonic modes on the ionic and thermal transport properties[4-6].

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IT-31

Designing Transparent Conducting Materials for Smart Devices through Band gap Engineering

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Abstract: Sustainability and environment friendliness are the two aspects the current research community is focussing on. In line with this, we have been working on designing and developing new systems and prototypes for smart wearables and displays based on non-toxic, earth abundant materials. In this talk I will be presenting our recent results in the area of designing transparent conducting materials through appropriate bandgap engineering for display devices. Transparent conducting materials are those systems exhibiting high electrical conductivity and high optical transparency-two seemly incompatible properties for conventional solid state materials, simultaneously. They form the back bone of electronics and optoelectronics industries including flat panel display devices, flexible touch screens, OLEDs, photovoltaic cells, smart windows etc. Decreasing the resistivity while maintaining the transparency in the layers is a trade-off relationship since it is difficult to achieve both the features simultaneously as the increase in the carrier concentration also leads to an increase in the visible absorption. Hence designing such materials requires a deeper understanding between the structure and the electro-optical properties, origin of the charge carriers, the dominant scattering mechanisms affecting the carrier mobility and hence limiting the performance. One possible way of achieving this is through band gap engineering through appropriate charge carrier doping, controlled defect generation and tuning the carrier mobility. In this talk we will discuss on the development and understanding of such transparent conducting materials-ITO and beyond.

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IT-32

ZnO: An Efficient Chemiresistive Gas Sensing Material of the Past, Present And Future

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Abstract: Metal oxide semiconductor (MOS) are among the most efficient sensing materials for realization of chemiresistive gas sensors[1-4]. This has predominantly attributed to the inherent characteristics of oxygen non-stoichiometry and high mobility of charge carriers[3]. This further enables the control over surface interactions crucial for gas sensing application. Among different MOS, ZnO in particular is looked upon as the best sensing material that has been widely studied in the past, present and holds the promise for future sensing applications also. The widespread utility of ZnO has been assigned to the numerous advantages that includes high sensitivity, stability, low cost fabrication, flexibility of synthesis, low power consumption, high temperature stability, and most importantly, simple gas sensing mechanism. In the past, the well establish chemistry of ZnO and ability to realize it in different forms namely pellets, thick and thin films has been utilized to achieve desired sensor configurations. At present, the recent advancement in nanoscience and nanotechnology has led to the numerous novel features that have found application in gas sensing. This includes wealth of interesting nano-morphologies, size and position control growth, complete understanding of growth mechanism and tuneable surface reactivity. Accordingly, different nanoforms especially pristine nanowires, nano-heterostructures and nanocomposites have been studied and utilized effectively to realize better sensing characteristics. In the similar context, for future sensor applications wherein it is envisaged the usage of IoT (internet of things) enabled sensors, increased potential of data handling and artificial intelligent, ZnO also holds the promise as the best sensing material. For example, ZnO nanowires have demonstrated excellent sensing properties when used as a multiple sensor array in an e-nose configuration for environment monitoring applications[5]. Thus, in the present talk, the evolution and the growth of ZnO as a sensing material will be emphasised taking help of literature and some of our own findings. Further, role of ZnO in the futuristic applications especially e-nose, wearable and self -powered sensors will also be discussed. Finally, some of the daunting challenges that needs to be addressed to realize the commercially viable sensors satisfying the stringent 4-S sensor selection criterion will also be addressed.

Keywords: ZnO; chemiresistive sensors; nanostructures; nanowires; e-nose; wearable sensors

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IT-33

Magnetic skyrmions and resonant spin excitation in two dimensions

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Abstract: Two-dimensional oxide interfaces provide a versatile platform to explore and engineer emergent properties such as superconductivity and novel magnetic order. The interface between two oxide compounds $La_{1-x}Sr_xMnO_3$ and $SrIrO_3$ supports the formation of a skyrmion crystal in the presence of an external magnetic field, due to competing ferromagnetic double-exchange coupling and Dzyaloshinskii-Moriya interaction present at the interface. The skyrmion crystal exhibits a finite scalar spin chirality which acts as a source of real-space Berry curvature, producing topological Hall effect. Furthermore, the dynamical structure factor, obtained from Monte Carlo simulations and Landau-Lifshitz dynamics calculations, reveal a very rich structure of resonant spin-wave excitation inside and in the vicinity of the skyrmion crystal phase. We identify a characteristic temperature T_s for a liquid-to-crystal like transition of the skyrmions. Above T_s for the skyrmion crystallization, a diffusive regime prevails in which topological spin texture of skyrmionic character starts to develop as the precursor of the skyrmion crystal. We discuss the opportunities for the detection of the spin waves excitations using inelastic-neutron-scattering experiments in manganite-iridate heterostructures.

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IT-34

Emergent many-body composite excitations and novel quasi particles of 1D quantum spin-1/2 trimer-chains

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Understanding exotic forms of magnetism in quantum spin systems is an emerging topic in modern condensed matter physics. Quantum dynamics can be described by particle-like carriers of information known as quasiparticles, which emerge from the collective behavior of the underlying system. In a conventional 3D magnet, the magnetic ground state is a long-range ordered configuration of the atomic magnetic moments, and the magnetic excitations are well described by the linear spin-wave theory with magnetic quasiparticles known as "magnons," carrying a spin-1.

On the other hand, the magnetic ground state of a 1D Heisenberg chain with $S = 1/2$ remains disordered even at absolute zero temperature, in contrast to its Ising counterpart, which becomes ordered only at zero temperature. Interestingly, the magnetic excitations of spin-1/2 Heisenberg chains are gapless and consist of exotic quasiparticles known as "spinons," carrying fractionalized spin-½. Such magnetic excitations cannot be accounted for by semiclassical spin-wave theory. In contrast, a non-uniform spin-1/2 chain, specifically, a quantum trimer spin chain with repeating exchange couplings J_1-J_1-J_2 (intratrimer J_1, and intertrimer J_2), exhibits qualitatively different magnetic ground states and spin excitations than its uniform counterpart. Our recent experimental neutron scattering results on naturally grown quasi-1D quantum spin-chain antiferromagnets [1-6] will be discussed to illustrate the microscopic magnetic correlations and their characteristic quasiparticle excitations. In particular, the recent discovery of emergent composite excitations of novel quasiparticles, doublons, and quartons in a quantum spin-1/2 trimer-chain antiferromagnet, imparting a strongly spin-entangled ground state, will be detailed.

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Contributory Papers

a) Phase transitions and dynamics

a0001

Spectroscopic and Luminescent Properties of Nickel doped $CaWO_4$

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Abstract. The effect of Nickel on the structural, optical and electronic properties has been studied via X-ray diffraction, Uv-Vis spectra and Photoluminescence spectra. For high concentration of nickel formation of secondary phase has been observed, and this phase needs to be identified. Bandgap has been observed to increase slightly for lower concentration of nickel and with further increase, bandgap decreased. With the inclusion of nickel in CaWO4 structure the broad emission peaks are observed between 300- 650 nm, which shows the possibility of modifying the PL towards white light emission.

a0002

Impact of nonic saturation on instabilities in Parity Time (PT)-symmetric Fiber Bragg Grating (FBG) structures

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Abstract: The effects of conventional nonic saturation on modulational instability are being studied in a Parity Time (PT) symmetric fiber Bragg grating structure (FBG) with various PT-symmetry regimes. A conventional linear stability analysis identified the modulational instability (MI) gain. Additionally, to investigate the MI in the FBG structure with PT symmetry when coupled effects such as nonlinearity and saturable nonlinearity are present. We find that the MI gain varies significantly due to nonic saturation. Finally, we show that, even in the presence of PT symmetry, effective control of the MI may be shown by varying the nonic and saturation nonlinearity for various PT-symmetric regimes. The investigation turns up several different spectrum kinds, including sideband spectrum, symmetry, asymmetry, steadily rising broad spectrum, gain, and others. We find an abnormal range that is more discrete than continuous for the few physical components. Following the application of PT - symmetry, the formation of solitons in nonlinear periodic structures is also examined.

a0003

Anharmonic Phonons and Anomalous Thermal Expansion in Vanadium Metal

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Abstract: Vanadium, an important metal in the alloy and steel industry, exhibits very large thermal expansion behaviour at high temperatures. In this work, we have extensively identified the role of phonons in the anomalous thermal expansion behaviour of vanadium, particularly at high temperatures. We have discussed the limitation of quasi-harmonic approximations (QHA) to predict the high-temperature thermal expansion behaviour in such a strongly anharmonic system. Our large-scale molecular dynamics (MD) simulations, which included all the anharmonic effects, successfully explained this anomalous behaviour.

a0004

Pressure Induced Amorphization in Pyrochlore $Gd_{1.99}Sm_{0.01}Zr_2O_7$ Compound

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The structural stability of Sm doped cubic $Gd_2Zr_2O_7$ (space group *Fd-3m*) compound with pressure has been studied by high pressure x-ray diffraction measurements using synchrotron radiation. The pressure-dependent x-ray data indicates that the ambient pyrochlore structure remains stable up to ~ 22.6 GPa. On further compression, all the diffraction peaks disappear, at ~36.6 GPa, only one broad hump is observed at 2θ ~10°. The experiment suggests a pressure induced amorphization initiated at ~24 GPa in the $Gd_{1.99}Sm_{0.01}Zr_2O_7$ compound. On release of pressure, a few weak diffraction peaks of ambient phase reappeared, implies to the partially reversible nature of the transition.

a0005

Disorder to Order Phase Transition and High Pressure Behavior of Sodium p-Nitrophenolate Dihydrate Crystal

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High pressure Raman spectroscopic investigations of sodium p-nitrophenolate dihydrate [$Na(C_6H_4ONO_2)$].$2H_2O$ (NPNa) is carried out up to 22 GPa. The present study indicates series of structural phase transitions at 0.7, 2, 6 and 15 GPa. The Intensity of Raman spectra vanishes drastically above 15 GPa. The visual observation through optical microscope indicated change of color from yellow to black in this pressure range indicating a change of the electronic structure in this compound. Comparing with reported temperature dependent study, the first high pressure transition (at around 0.7 GPa) is identified as disorder to order phase transition. On pressure release from 22 GPa we could not detect any Raman signal in the recovered sample indicating irreversible nature of the high pressure transition.

a0006

Synthesis of Lutetium Dihydride at HP-HT and its relevance to the N-doped superconducting lutetium hydride

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Abstract. Recent discovery of room temperature superconductivity in the nitrogen doped lutetium hydride ($LuH_{3-\delta}N_{\varepsilon}$) (SNLH) has stimulated the interest in the synthesis of lutetium hydrides and their detailed understanding. Phase pure LuH_2 has been synthesized using pure Lutetium (Lu) metal and Paraffin as hydrogen source at high pressure and high temperature conditions. The sample inside diamond anvil cell (DAC) has been characterized with optical micrographs using high resolution optical microscope. The recovered sample is characterized using synchrotron based angle dispersive x-ray diffraction (ADXRD) measurements. Comparison of high pressure evolution of the unit cell volumes of synthesized LuH_2, SNLH and cubic phase of LuH_3 provides insight about the composition and structure of reported SNLH. Data analysis at high pressures reveals that the parent framework for reported SNLH compound is LuH_2 rather than LuH_3. The detailed stoichiometry of this compound is determined to be as $LuH_{2+x}N_{\varepsilon}$.

a0007

Response of Bismuth under Planar Dynamic Loading

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Plate impact and shock recovery experiment conducted on polycrystalline bismuth (Bi) material at single-stage light-gas gun facility at BARC to understand its response under dynamic loading to 10.23 GPa. In two separate plate impact experiments, one designed for in-situ measurement of dynamic loading profile and other configured for recovery mode, the sample was subjected to dynamic pressure above ~10.23 GPa. The multi wave structure of free surface velocity (FSV) history of the sample recorded during passage of shock wave indicates two structural phase transitions one around 2.39 GPa and other around 7.9 GPa. The observed phase changes appear to be reversible as indicated from XRD patterns of as received and shock treated samples from both the experiments. Also, the mechanical strength properties have been determined from recorded FSV profile.

a0008

Predictions of New compositions of Thorium oxides under pressure: Ab-initio study

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Due to their prospective applications as advanced nuclear fuels, thorium oxides have been the topic of intense studies. The phase diagram of the Th-O scheme, however, continues to be unknown at low temperature and extremely high pressure. In present work, we examine the phase diagram Th-O system up to 300 GPa resorting the first-principle band structure method along with evolutionary structure search algorithm. Apart from the experimentally observed compound (ThO_2), several other chemical stoichiometries (ThO, ThO_3, ThO_4, and Th_3O_5) are found to have stability fields on the Th-O phase diagram at pressure of 27 GPa, 20 GPa, 250 GPa and 180 GPa, respectively. Further, the structural stability of each predicted composition has been examined with pressure from free energy point of view and substantiated by lattice dynamical stability analysis.

a0009

Vortex Nucleation and Feynman Rule in Double-Well Confined Bose-Einstein Condensates with Density-Dependent Gauge Potentials

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A rotating Bose-Einstein condensate, when confined in a double-well potential, not only gives rise to visible vortices but also produces hidden vortices. We have empirically developed the Feynman's rule for the number of vortices vs angular momentum in case of Bose-Einstein condensates subjected to density-dependent gauge potentials. Though the Feynman rule is satisfied only when both visible and hidden vortices are taken into account. However, the variation of the average angular momentum with the number of vortices is also sensitive to the nature of density-dependent gauge potential and the peak density of the condensate. The empirical result agrees well with the numerical simulations. In addition, we show the nucleation of vortices in Bose-Einstein condensates with nonlinear rotations alone (without any trap rotation) arising through the density-dependent gauge potential.

a0010

Temperature Dependent Vibrational Studies of $ZnNb_2O_6$

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In the recent past binary metal oxides of the type AB_2O_6 (*A* is divalent cation: Zn, Mg, Ca, Cu, Mn and *B* is pentavalent cation: V, Nb, Ta) has shown potential application as the battery storage materials, capacitors, microwave electronic devices, etc. $ZnNb_2O_6$ is one such compound, which is technologically important material. In this work, we report the temperature dependent vibrational properties of this compound from 78 K to 873 K using Raman spectroscopy. Appearance of new modes at ~ 493 K suggests the presence of phase transition in the compound.

a0011

Phase Transition Studies on $TbNbO_4$ using in-situ Raman Spectroscopy

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Rare earth niobates have shown a significant interest in the research community due to their diverse properties and potential applications. $TbNbO_4$ stands out as a member of the niobates family that exhibits properties suitable for optical applications and various other uses. While earlier research has focused on high-temperature X-ray diffraction (XRD) studies on $LaNbO_4$, which revealed a well-known monoclinic to tetragonal phase transition. Due to its technological importance, this compound is also required to study under non-ambient conditions. Thus, the present study's aim is to investigate the behaviour of $TbNbO_4$ at different temperatures ranging from 78 K to 873 K using in-situ Raman Spectroscopy. This study suggests a complete phase transition in the compound from 613 K to 673 K.

a0012

***Ab initio* Calculations on High Pressure Phase Transition of Titanite ($CaSiTiO_5$)**

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Titanite ($CaSiTiO_5$) is one of the common accessory minerals in the magmatic and metamorphic rocks. Several of naturally occurring minerals suffer phase transition at extreme conditions. According to the experimental observations, titanite also undergoes a phase transition from $P2_1/c$ to $C2/c$ phase at high pressure and temperature. However, there is a scarcity of high pressure phase information beyond 7 GPa. In this article, we have explored high pressure response of titanite up to 40 GPa from ab-initio calculations. Our calculations indicate two different types of structural phase transition at 20 GPa and 34 GPa. We infer that phase transition at 20 GPa has the feature of second order whereas it is of first order at 34 GPa. The isolated SiO_4 tetrahedra in low pressure titanite transforms into interconnected SiO_6 octahedra around the onset of first order phase transition.

a0013

Higher Order Phonon Anharmonicities and lattice thermal conductivity in bulk $MoSe_2$ and WSe_2

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Abstract: Using inelastic neutron scattering and X-ray diffraction measurements, together with ab-initio and machine-learned molecular dynamics simulations, we bring out the role of higher order anharmonicity in the phonon spectra of $MoSe_2$ and WSe_2 relevant to thermal transport and thermal expansion behaviour. We show that the perturbation method, including 4th-order force constants, is insufficient to capture the temperature-dependent explicit anharmonicity. The Green-Kubo method captures the explicit anharmonicity and reproduces the thermal conductivity (κ_l) with high fidelity. Our mode-resolved calculation reveals that the major contribution to κ_l is attributed to a small explicit anharmonicity of low-energy phonons.

a0014

Unraveling Interactions between Ionic Liquid and DPPC Membrane

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In this work, we present a comprehensive molecular dynamics simulation to investigate the effect of 1-decyl-3-methylimidazolium bromide ionic liquid (IL) on the dipalmitoylphosphatidylcholine (DPPC) membrane in aqueous solution. Below 314 K, DPPC molecules forms gel phase characterized by highly ordered alkyl chains, with fewer gauche defects and small area per lipid (APL). The gel to fluid main phase transition of bilayer is captured well in our simulations at ~ 314 K, consistent with differential scanning calorimetry experiment. The fluid phase features disordered alkyl chains, higher gauche defects and a large APL. Interestingly, the presence of ILs minimally affect the gel phase, indicating limited insertion into the bilayer, and majority self-aggregating into micelle-like structures. However, ILs alter the phase behavior, leads to an early onset of the phase transition at 310 K. In the fluid phase, ILs stop aggregating, allowing more insertion into the bilayer and increasing APL. The early transition is due to weakened Van der Waals interactions between lipids induced by ILs. Our study provides microscopic insights on IL destabilizing the cell membrane across various phases.

a0015

Optimization of dyes using different donors for dye-sensitized solar cell applications – A Computational analysis.

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Abstract: Methoxy (OCH_3) substituted carbazole, diphenylamine and triphenylamine based Donor -π-Spacer - Acceptor type organic sensitizers are investigated by density functional theory (DFT) and time-dependent density functional theory (TD-DFT). Carbazole, diphenylamine and triphenylamine are used as donor moiety. Cyanovinyl and furofuran are used as π-spacers subunits and benzoic acid was used as an acceptor moiety. The essential properties of organic dyes such as optical and Frontier molecular orbital analysis are dye-sensitized sensitized solar cell (DSSC) application. The highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbitals (LUMO) are obtained from the optimized geometry. The optical property and light harvesting efficiency are analyzed by TD-DFT calculation. The results reveal that the length of the π-spacer unit and different donors in the organic dyes could improve the sensitizer's properties.

a0016

Structural Phase Stability and Surface Chemical State of $Fe_{2-x}Sc_xO_3$ System (x=0.2, 0.5, 1.0)

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We report the synthesis and structural phase stabilization of the $Fe_{2-x}Sc_xO_3$ system by mechanically alloying of α-Fe_2O_3 and Sc_2O_3 metal oxide. Powder X-ray diffraction (XRD) patterns confirmed the single-phase rhombohedral structure with space group R-3c for x=0.2 ($Fe_{1.8}Sc_{0.2}O_3$), mixed phase in $Fe_{1.5}Sc_{0.5}O_3$ (x=0.5), and single-phase cubic structure with space group I-a3 for x=1.0 ($FeScO_3$) at subsequent heat treatment range 800-1300° C. X-ray photoelectron spectroscopy (XPS) was employed to investigate the electronic charge states of the Fe and Sc ions. Fe 3s XPS spectrum showed a doublet peak, deviating from the anticipated singlet peak behavior predicted by the spin-orbit coupling theory, suggesting the presence of magnetic interactions within the system. This anomalous behavior is considered to be of magnetic origin. The structural phase stabilization of the samples depends on the amount of metal oxide (Sc_2O_3) and sintering temperature.

a0017

Investigation of Topological Phase Transition in Non-centrosymmetric LiCaBi Compound: A First-principles Study

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The Non-centrosymmetric materials offer an exciting opportunity to discover a diverse range of topologically intriguing compounds. By leveraging the tunability of their hybridization strength through lattice parameters, we investigate the potential of achieving a topological insulating phase in the novel LiCaBi compound using the *first-principles* calculation within the framework of density functional theory. The dynamical and mechanical stabilities of the LiCaBi are investigated by the phonon dispersion curves and elastic constants, respectively. The LiCaBi compound exhibits a semi-conducting nature with direct band gap of 0.59 eV. We have applied volume expansive pressure (VEP) to engineer the band topology of material which leads to -*s*-p_z orbital inversion around the G point having primarily indication from trivial to non-trivial phase transition. At 8.4% VEP with spin orbit coupling (pressure of ~5 GPa), the LiCaBi undergoes topological phase transition with non-trivial energy gap of 64 meV. Our results show that the LiCaBi could be a potential candidate for the practical application in the field of spintronics and nano-electronics.

a0018

Critical analysis of half-metallic Heusler Co_2TiSi

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We have investigated the critical analysis/phenomenon of the half-metallic full-Heusler Co2TiSi across the transition temperature (TC) associated with the ferromagnetic second order phase transition. The analysis following modified Arrott plot method, Kouvel-Fisher technique, and critical isotherm plot suggests the critical exponents as β=0.368, γ=1.15, and δ=4.13 with TC 380 K. The self-consistency and reliability of the obtained exponents are further verified by the Widom scaling relation and scaling equation of states.

a0019

Lattice Vibration Study of a Distorted Bismuth Substituted $SrFe_{12}O_{19}$ Compound

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The polycrystalline $Sr_{1-x}Bi_xFe_{12}O_{19}$ (x = 0, 0.01, and 0.02), prepared through the sol-gel auto-combustion method has created significant lattice distortion at 12k- sites. The Raman spectra of SBFO1 (x = 0.01) show that SBFO1 is the highly strained system as compared to the x = 0 & 0.02 and its 2b &12k site is the most distorted site; resulting in 417.7 cm^{-1} Raman peak of SrM (x = 0) associated with 12k-site split into two peaks at 413.8 cm^{-1} and 432.9 cm^{-1} for x = 0.01. The low damping constant of SBFO1 also satisfies the highest compressive nature of SBFO1 as observed in XRD. The Raman peak shift shows an analogous result as the bond length associated with different sites.

a0020
High Pressure Raman Scattering Studies on CuV_2S_4
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Thiospinel, CuV_2S_4, is a unique system with three dimensional charge density wave (CDW) and narrow band metallic states. Here, in this study, we have performed Raman scattering experiments on CuV_2S_4 at high pressures up to ~13.6 GPa. Data analysis of Raman spectra shows that this compound undergoes two transitions at 0.3 GPa and 3.0 GPa to new high pressure phases. The first high pressure phase shows signatures of electronic rearrangement possibly imitating the phase with presence of CDW. The new phase beyond 4.6 GPa could be characterized as the low symmetry phase with virtue of Raman mode splitting. This phase would have correspondence with the orthorhombic phase observed at very low temperatures. On release of pressure, it does not come back to parent phase implying its irreversible nature.

a0021
Tailoring Optical Properties of E-Beam Evaporated Vanadium Oxide Thin Films for Smart Window Application
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Vanadium dioxide (VO_2) exhibits reversible change in carrier density at 68^0C due to insulator to metal structural phase transition with distinctive change in optical and electrical properties in the presence of heat, light, and strain. In this work, the optical and thermochromic properties of the electron beam evaporated vanadium oxide (VO_x) thin films deposited at different oxygen flow rates have been investigated by analyzing spectroscopic transmission and ellipsometry data of the films measured at different temperatures. The absorption loss in the films is found to be decreasing with increasing oxygen flow rate. It is shown that the thermochromic properties of the VO_x films can be tailored by varying the oxygen partial pressure without any post deposition annealing treatment.

a0023
Suppression of Phase Transition in Single Crystal Aluminium by Double-Shock Compression
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Despite numerous dynamic compression experiments there remains a lack of clear understanding and quantitative data on shock-induced structural phase transition of elemental Al. Through extensive non-equilibrium molecular dynamics simulations, recently for the first time, we have shown that shock-induced fcc to bcc phase transitions in single crystal Al along [001] direction triggers at 30 GPa, which is one order magnitude less than room temperature static and ramp compression values. The current paper is an effort towards examining phase transformation dynamics of single crystal Al under double-shock compression. It is shown that for two successive shocks with certain strength ratio, the extent of bcc conversion can be significantly suppressed by tuning the time delay between the pulses. Moreover, slowing down the compression dynamics in double-shock pulse facilitates near-constant bcc phase-fraction over a longer period of time than single-shock method.

a0024
High Temperature Raman Spectroscopic studies on $LiNiPO_4$
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Olivine structured $LiNiPO_4$ is potential cathode material in Lithium-ion batteries due to its high energy density. In the present work, we report synthesis of olivine structured α- phase $LiNiPO_4$ using ceramic method and its vibrational behavior under high temperature using Raman spectroscopic technique up to 873 K. As the temperature is increased, all the Raman peaks are

found to show red shift due to obvious lattice expansion along with thermal broadening, however compound remains in α-phase up to the highest temperature reached in present studies. All the observed changes are found to be reversible.

a0025

Phase Transition Studies in $CsCuCl_3$ under Hydrostatic High Pressure Conditions

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Abstract. Hexagonal perovskite caesium trichlorocuprate ($CsCuCl_3$) has been studied through synchrotron x-ray diffraction and Raman spectroscopy techniques under hydrostatic high pressure conditions up to 11.25 GPa. $CsCuCl_3$ is observed to undergo complete phase transition at pressure 2.59 GPa. The peaks which are observed separate (~ 156 cm^{-1} & 177 cm^{-1}) in ambient condition are merged into single peak (~ 194 cm^{-1}) under high pressure condition. This effect has been correlated with stretching of bands in $CsCuCl_3$. Similarly peaks (~ 265 cm^{-1} & 286 cm^{-1}) correspond to A_1 and E_1 modes respectively are disappeared after phase transition (PT). New peak evolved (~287 cm^{-1}) corresponding to $1E_{2g}+1A_{1g}$ mode of distorted phase. These results are supported with reduction in lattice parameters and appearance of new peak corresponding to distorted phases as observed in X-ray diffraction. Finally after releasing the pressure both Raman and XRD measurements show similar spectra as of ambient which confirms the phase transition is reversible in nature.

a0026

Modulation of Skyrmion Phase by Doping in Cu_2OSeO_3

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Over the last decades, skyrmion hosting systems have attracted researchers for their rich physics and potential applications in spintronic devices. Here, we report the change in the structural and magnetic properties in skyrmion hosting Cu_2OSeO_3 upon doping of magnetic (Ni^{2+}) and nonmagnetic (Zn^{2+}) ions. The room temperature X-ray diffraction confirms pure cubic B20 phase of all three systems, i.e., Cu_2OSeO_3, $Cu_{1.8}Ni_{0.2}OSeO_3$ and $Cu_{1.8}Zn_{0.2}OSeO_3$. It is realized that Dzyaloshinsky-Moriya interaction weakens upon Zn doping and strengthens upon Ni doping in Cu_2OSeO_3. Moreover, fluctuation disordered phase is observed to be persistent in the parent as well as doped (Ni and Zn) Cu_2OSeO_3 indicating that it is indeed a precursor phase for the stabilization of helimagnetic phases. The variation of magnetization is almost similar in Cu_2OSeO_3 and $Cu_{1.8}Zn_{0.2}OSeO_3$, however, Ni doping shows rich physics when compared with Cu_2OSeO_3.

a0027

Effect Of Eu^{3+} Doping In $Y_2Ge_2O_7$ Under Pressure

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High pressure (HP) x-ray diffraction (XRD), Raman scattering and photoluminescence (PL) experiments have been performed on tetragonal structure (S.G. $P4_32_12$) of $Y_{1.8}Eu_{0.2}Ge_2O_7$ (YGOE). High pressure PL studies shows existence of multiple non equivalent sites for Eu3+ ions, suggested by splitting of $5D_0 \rightarrow 7F_0$ and appearance of additional lines at $5D_0 \rightarrow 7F_1$ transitions band in the emission spectra. Asymmetric ratio is gradually decreased to a much smaller value suggesting some structural transformation leading to symmetric environment in the neighbourhood of Eu^{3+} ion. The HP Raman studies on $Y_{1.8}Eu_{0.2}Ge_2O_7$ suggest that the signature mode of pyro group slowly disappears around ~15 GPa indicating coordination polyhedra, GeO_4 has been changed. Broad Raman mode corresponding to asymmetric stretching vibration of GeO_3 polyhedra shows negative pressure coefficient suggests increase in Ge coordination number. High pressure x-ray diffraction (XRD) indicates that tetragonal phase of YGOE undergoes concomitant crystalline to crystalline and amorphous phase transition between the region 14-18 GPa. The high pressure crystalline phase may be distorted pyrochlore type structure. The transformation is irreversible upon release of pressure.

a0028

Pre-melting Behavior of O-phthalic Acid-A Raman Scattering Study

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Abstract. The vibrational spectra of hydrogen-bonded molecular crystals are of importance in the context of understanding the role of hydrogen bonds in the thermodynamic properties of these systems. Raman scattering studies of ortho-phthalic acid, (benzene-1,2-dicarboxylic acid) have been carried out up to 240 ºC and its pre-melting behavior is discussed.

a0029

Studies of lattice dynamics in $Na_2Ni_2TeO_6$

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$Na_2Ni_2TeO_6$ is a sodium-containing novel layered honeycomb oxide for solid state battery cathodes, made possible due to the high migration of Na^+ ions. The vibrational properties of this material were investigated using potential model calculations. The reported Raman spectroscopic data are in good agreement with calculations. Molecular dynamics simulations with increasing temperature indicate large mean square displacement of Na as compared to other constituent atoms. Pair-correlations between various atom pairs were also computed.

a0030
Temperature dependent Structural phase transitions in Binary Solid solutions 0.30 $NaNbO_3$-0.70 $Na_{0.5}Bi_{0.5}TiO_3$
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Abstract. The solid solution of 0.30 $NaNbO_3$-0.70 $(Na_{0.5}Bi_{0.5})TiO_3$ has been synthesized and investigated to explore its structural phase transitions with temperature using X-ray diffraction. Our analysis reveals distinct changes in the powder diffraction data, including the appearance and disappearance of super lattice reflections and alterations in the primary perovskite peaks. These observations suggest temperature-driven structural phase transitions. Through Rietveld refinement, we demonstrate that the material exhibits a coexistence of the ferroelectric rhombohedral R3c phase from pure NBT and the antiferroelectric tetragonal P4bm phase within the temperature range of 10K to 598K, featuring varying phase fractions. Beyond 598K, a transition to a single phase antiferroelectric P4bm, resembling to pure NBT, is observed. Notably, at temperatures surpassing 723K, a complete transformation into the high-symmetry cubic phase with space group Pm3m occurs. Detailed results are discussed

a0031
High Pressure Behavior of Energetic Material Dinitrotoluene
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High pressure behavior of 2,4-dinitrotoluene (DNT), an energetic material, was studied using Raman spectroscopy up to ~19 GPa. Qualitative changes are noted in the Raman spectra around 3 GPa and 7 GPa indicating possible phase transitions in the compound at these pressures. Above 13 GPa, intensity of many of the Raman bands reduce rapidly, accompanied by broadening. Spectral features of DNT molecular unit persisted up to the highest pressure reached, namely 19 GPa.

a0032
Structural, Dielectric And Thermal Stability In Sm^{3+} Modified $SrBi_4Ti_4O_{15}$ Piezoelectric Ceramics
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Abstract. $SrBi_{4-x}Sm_xTi_4O_{15}$ (x=0.00, 0.05, 0.1, .0.15, 0.2) bismuth layer structure ferroelectric ceramics were prepared by a solid-state reaction route. X-ray diffraction technique suggested that all compositions have orthorhombic structure with $A2_1am$ space group. Dielectric study reveals that both dielectric permittivity and phase transition temperature reduces with increasing Sm^{3+} content. In addition to that lower tangent loss and thermal stability was achieved in the Sm - modified composition, which is related to the oxygen vacancies mechanism. All the result indicated that the prepared ceramic is a suitable candidate for high temperature piezoelectric application.

a0033
Glass Transition in Dense Thermo-responsive Microgel Suspensions: A Monte Carlo Study
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Abstract. Identification and characterizing the glass transition in monodisperse dense colloids of soft sphere systems is of considerable interest in view of their commonality with atomic systems. As well their numerous applications in diverse fields. Among the various colloidal systems, Poly (N-isopropyl acrylamide) (PNIPAM) microgel suspensions have garnered significant attention due to their responsive nature to external stimuli such as temperature (*T*), Pressure (Osmatic) and *pH*. PNIPAM microgel are core and shell structured soft spheres undergo reversible volume changes in response to changes in temperature. This thermo-responsive behavior allows researchers to tune both particle size as well as interparticle interactions by varying *T*. In this study, we employ Monte Carlo (MC) simulations to investigate the glass transition phenomena in dense PNIPAM microgel suspensions, by employing the recently proposed multi-Hertzian (MH) [1] pair potential. The glass transition is investigated by quenching the microgel liquid like order state ($T = 30^0$C) to temperature much below its freezing transition into ordered state ($T < 22^0$ C). The glass transition temperature is identified by calculate structural parameter Revache parameter R_g, and also structural and dynamical parameters across the glassy transition. We report here for the first time

occurrence of glass transition in dense PNIPAM microgel suspensions despite the particles being mono-dispersive in size. The glass transition occurs due to kinetic arrest of PNIPAM microgels.

a0034

Lattice dynamics study of semiconductor mixed crystal wurtzite $Zn_{1-x}Mg_xS$

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Abstract. We present a study of the structural and lattice dynamical properties of wurtzite phase of ZnS, $Zn_{1-x}Mg_xS$, and MgS, employing shell model calculations. Our calculations incorporate the treatment of disorder through a supercell approach. The calculated lattice constants for different concentrations, as well as the phonon frequencies at the Brillouin zone centre are in good agreement with previous experimental and theoretical results.

a0035

Hugoniot of Porous Copper up to 300 GPa using First-Principle Calculations and Enthalpy-based Equation of state

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Hugoniot of porous copper at different initial porosities (1, 2, 3 and 4) up to 300 GPa pressure have been calculated employing first principle calculations and enthalpy-based equation of state (EOS). First, static energy, pressure and enthalpy at T=0 K were obtained using PWSCF code. The zero kelvin isotherm follows available experimental data at ambient condition. The cold components of energy (E_c), pressure (P_c) and enthalpy (H_c) have been employed to evaluate enthalpy parameter (χ_H) along the Hugoniot of normal Cu. Then shock Hugoniot, shock and particle velocities at various porosities were computed using χ_h. Here, theoretical findings agree well with experimental data.

a0036

Multiple magnetic phase transitions exist in the bilayer manganite La_(1.4)Sr_(1.6)Mn2O7.

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Abstract. Bi-layer La_1.4 Sr_1.6 Mn_2 O_7 exhibits three magnetic transitions at 101 K, 246 K, and 295 K (through M-T curve). Because conducting and insulating regions have greater and lower ordered magnetic states, respectively, the magnetic and metal-insulator transitions at 101 K suggest that there is a close connection between magnetic and transport features.

b) Soft matter including polymer and biological systems

b0001

Self-activated Fluorescence Induced By Oxygen Vacancies In Hydroxyapatite: A Biological Perspective

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Abstract. Polymorphic hydroxyapatite (HAP) with 54.34 vol.% monoclinic ($P2_1/b$) and 45.66 vol.% hexagonal ($P6_3/m$) is synthesized and its properties are reported. The polymorphic HAP contains oxygen (O) vacancies that is intricately linked with its ability to show fluorescence at 532.9 nm. The details of O vacancies were obtained primarily from the x-ray photoelectron spectroscopy (XPS) and reconfirmed by the electron spin resonance (ESR) spectra that peaked at a Landé g-factor of 2.003. These defects created electronic energy levels in the forbidden gap, facilitating the electron-hole recombination for showing fluorescence. These events strongly point towards engineering the processing conditions to tune the optoelectronic property that has enormous technological implications.

b0002

Response Of Liquid Crystals To An Oscillating Electric Field

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We performed Monte Carlo simulations on a liquid crystal system using a lattice spin model in three dimensions to study the behavior of order parameter (ρ) in presence of an oscillating electric field. Hysteresis is observed when we plot order parameter against the electric field. The area of this hysteresis loop increases with the increase in frequency (ω) of applied field up to a certain frequency ω^† and decreases and goes to zero if frequency is increased further. We find that the area of the loop scales as AE^α ω^β/(B^2+ω^(1+γ)) with exponents α=0.75, β=0.5 and γ=0.75.

b0004

Influence Of layer Sequence On Near Edge Structure And Morphology In PS and PMMA Bilayers

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Abstract. The observations of X-ray Absorption Spectroscopy (XAS) (in the near edge region) and atomic force microscopy (AFM) on PS/PMMA/FG (float glass) and PMMA/PS/FG bilayers are reported here. The bilayers were prepared by spin coating technique at a speed of 5000 rpm. For reference, bulk PMMA was also used. X-ray absorption in the near edge region of carbon and oxygen elements of the polymers showed changes in the features and their respective intensities when the layer structure was reversed, although the absorption energies match well with that of bulk PMMA. Corresponding AFM images exhibited drastic change in the top surface morphology when PMMA was used as an upper layer and exhibited fiber like structure along with pits and island like growth. The observed results are expected to improve the current knowledge of this immiscible polymer system, which has till date been mainly and extensively studied in blend form.

b0005

Understanding Correlation between Diffusion and Bond Lifetime in Deep Eutectic Solvents

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In recent years, aqueous-based deep eutectic solvents (DESs) have emerged as a subject of interest for customizing the physicochemical properties of pure DESs. However, the addition of water disrupts the extensive hydrogen bond network and complexes between species, raising questions about its impact on diffusion mechanisms. In this study, we used classical molecular dynamics (ND) simulations to explore the role of water in understanding the diffusion mechanism of acetamide in aqueous mixtures of acetamide and lithium perchlorate-based DESs, covering a wide range of water concentrations. Our findings reveal that water significantly alters the diffusivity of acetamide, with dynamics strongly governed by hydrogen bond and complexation lifetime. A power law scaling relationship is established between the acetamide diffusion coefficient and bond lifetime, highlighting their correlation. Notably, a threshold value of approximately 20 water wt. % separates two distinct regions corresponding to different diffusion mechanisms. This work provides valuable insights into the interplay between water and the diffusion behaviour of acetamide in DESs.

b0006

Solvent Induced Aggregation of Colloids in Confined Geometry

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Abstract. Interparticle interaction plays crucial role in governing stability of colloidal dispersion and it can be tuned by changing the physicochemical conditions, such as temperature, pH, solvent modification etc. Aqueous dispersions of nano-silica, stabilized by alkali ions, in basic environment can be de-stabilized by partial replacement of solvent . Scattering measurements provide in-depth quantitative aspects of structural modifications due to such destabilization process. In this work, we report synchrotron-based scanning-SAXS experiments in a confined geometry by partially replacing the continuous polar phase by non-polar alcohol solvent. A non-monotonic behavior of structural correlation at mesoscopic length scale was found with respect to alcohol/water ratio (R_{aw}). While ramified fractal-like correlation is manifested at intermediate values of R_{aw}, the structural correlation reappears with enhanced ordering at regimes of higher R_{aw}. Inter particle interactions shifts from repulsive to attractive type under uptake of stabilizing alkali ions by RO⁻ part of alcohol. This work indicates the possibility of formation of colloidal glasses at high R_{aw} regime and opens the possibility of particle dynamics simulation with varying attractive and repulsive contributions of potentials defining colloidal stability.

b0007

Rigidity Of Lamellar Lipid Membrane and It's Control

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We have shown the importance of rigid forces between adjacent components in lipid molecules in the formation of the lamellar bilayer phase through NVT Monte Carlo simulations on the simplest three-atom model of the lipid molecule including the solvent. We have also shown how the rigidity in monolayers and trilayers of DPPC can be controlled by introducing Na and K ions in the aqueous subphase. The monolayer is found to be most sensitive to ionic changes and the trilayer has the maximum bending strain at Na/K = 50/50.

b0009

Reverse Hofmeister Effect on Bilayer Adsorption of Lysozyme

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Abstract. Lysozyme (LSZ) is a cationic protein below the isoelectric point (IEP ≈ pH 11.2) and its solubility varies in accordance with reverse Hofmeister series in environment with low or moderate concentration of ions. The current study comprises bilayer films of LSZ, stabilized on hydrophilic silicon (Si) surfaces via dipping method and the study of reverse Hofmeister effect on these adsorbed films modified by mono-(Na^+), and di-(Ca^{2+}) valent ions. Atomic force microscopy (AFM), X-ray reflectivity (XRR) and water contact angle (CA) techniques were applied to study the topographical, structural and wetting properties of the LSZ films modified by Hofmeister ions. Thick bilayers of LSZ molecules are adsorbed in presence of mono- and di-valent Hofmeister ions. The bilayer of LSZ formed on Si surface contains a bottom layer of LSZ, attached to the substrate in side-on alignment and one more layer of LSZ stabilized on top of that in side-on alignment or tilted alignment with reference to bottom layer. The thickness, RMS roughness as well as CA of LSZ films modified by ions obey the reverse Hofmeister series.

b0010

Mixing Demixing Of A Phase Separated Binary Colloidal System In An External Modulation

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We explore the rich phase behaviour shown by a binary phase separated colloidal system under external spatially periodic modulation. We perform Monte Carlo simulation on a binary mixture of big and small repulsive Lennard-Jones particles with diameter ratio 1:2. We characterize structure by isotropic and anisotropic pair correlation function, cluster size distribution, bond angle distribution, and demixing order parameter. We observe that there is a tendency of mixing among the two species under external modulation which gets enhanced with increasing potential strength. The smaller particles tend to form hexagonal order among themselves, as reflected in bond angle distribution after being subjected to external modulation. The phase transition from demixed to mixed state is observed through the demixing order parameter and the specific heat. On a reverse scenario, when we start from a mixed state and switch the external modulation off, then we observe that sizes of the clusters of smaller particles grow in time and the phase separated state returns as the system evolves in time.

b0011

Positron Annihilation Lifetime Study on Chloroinated Zeolitic Imidazolate Frameworks (COK-17): An in situ Observation of Pore Volume Evolution during CO2 Adsorption

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Abstract. COK-17 is a new form of flexible zeolitic imidazolate framework [Zn(4,5-dichloroimidazolate)$_2$] with the sodalite (SOD) framework topology having open-pore structure providing unique adsorption sites for selective gases. Thus COK-17 is

a promising candidate for natural gas purification through the adsorption of greenhouse gases. Positron annihilation lifetime measurements have been carried out to investigate the modifications of pore architecture in the COK-17 framework under varying pressure of CO_2 at room temperature. Interestingly, a long positronium lifetime component is observed to appear at CO_2 pressure around 10bar. The appearance of the long lifetime component indicates the evolution of large voids due to conformational transition in the extended framework of COK-17 at high pressure of CO_2. The creation of voids as a result of the conformational changes above 10 bar possibly be caused due to severe twisting of dcIm (dichloroimidazolate) linkers and tilting of ZnN_4 tetrahedra at high gas pressure.

b0012

The Effect Of Protein Binding On Conformational Stability And Order Of DNA Duplex With Hoogsteen Base Pairing

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Hoogsteen base pairing is an alternative base-pairing scheme in DNA double helices [1]. The Watson-Crick (WC) and Hoogsteen (HG) base pairs (bps) for A-T are sketched in Fig. 1. Several experimental studies have shown that the HG bp is stabilized in presence of proteins. We use conformational thermodynamics [2] to investigate the stability of a HG bp containing duplex DNA at the molecular level in the absence and presence of proteins. We study three different systems: (i) WC, a model system of DNA; (ii) HG, HG bp containing DNA; and (iii) HGP, HG bp containing protein-bound DNA. We compute conformational thermodynamics data for each bp: (i) in the HG system and (ii) in the protein-bound HGP system, both with respect to the WC system. We observe that, in contrast to the WC bp, the HG bp is flexible in the bare DNA duplex, but it is stabilized and organized in the HGP system [3]. The backbone torsion angles of bp fluctuate less to stabilize and organize the HG bp. We apply well-tempered metadynamics [4] to the aforementioned three systems and find that HG bp is about 3 kcal/mol less stable than WC bp in the absence of proteins, whereas it is about 3 kcal/mol more stable in the presence of proteins [5].

b0014

Langmuir Monolayer of Protein (Lysozyme)-Lipid (DMPA) Complex at Air-Water Interface

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Abstract. Langmuir monolayer of Lysozyme-DMPA complex as well as the pristine monolayer of DMPA is formed at the air-water interface having subphase pH ≈ 7.0. Surface pressure (π) - specific molecular area (A) isotherms are recorded for complex as well as pristine DMPA monolayer to investigate the effect of individual on the phases and phase transition occurring with monolayer compression. The difference in π–A isotherm of lysozyme-DMPA complex monolayer from that of pristine DMPA indicates the possible occurrence of interaction among protein (lysozyme) and lipid (DMPA) molecules, which results in showing different phases macroscopically. Morphological features of the protein (lysozyme)-lipid (DMPA) complex film is explored at the air-water as well as at air-solid interface using Brewster angle microscopy (BAM) and Atomic Force Microscopy (AFM) respectively. Variation in morphological features of protein-lipid complex film is probably due to the hydrophobic and electrostatic interaction occurring between oppositely charged lysozyme and DMPA molecules.

b0015

Theoretical Investigation on the Interaction of Nucleobases-Decorated Graphene Quantum Dot

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Using cutting-edge first principles methods based on density functional theory, we concentrate on the development of a benignly peculiar cluster like pristine GQD (Graphene Quantum Dot) and GQD containing nucleobases like uracil (U), cytosine (C), adenine (A), thymine (T), and guanine (G). Investigations into the most stable configuration for the adsorption of various nucleobases also revealed riffs in the structure and adsorption properties of GQD in response to the binding of nucleobases. According to the predicted adsorption energy, GQD and GQD containing nucleobases should adsorb in the following order, as follows: C > T > A > U > G. The estimated adsorption energies suggest that nucleobases adsorbed on GQD may be an elite choice for biosensor design. This strengthens the use of GQD for the detection of the aforementioned biomolecules. Understanding the nanointerface was also important for studying the effects of several graphene-related compounds, notably GQD, on live cells and human health. Additionally, it was helpful for illuminating potential sequencing maneuvers.

b0016

$Mg(NO_3)_2$ Doped Chitosan:Dextran Polyblend Electrolytes for Solid State Battery Application

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All solid-state batteries are garnering attention in both academia and industry. In the past few years, there has been a notable surge in the exploration and investigation of solid biodegradable blend polymer electrolytes (SBPE) due to their renewable and eco-friendly characteristics. A polymer electrolyte system was made by combining chitosan and dextran in a 60:40 ratio, then doping it with different concentrations of magnesium nitrate salt. The solution casting technique was used to prepare the system, using 1% acetic acid as the solvent. The prepared material is a free-standing film which is suitable for flexible device fabrication. The physical and chemical properties of SBPE were investigated using three techniques: X-ray diffraction (XRD), Fourier transform infrared (FTIR), and electrochemical impedance spectroscopy (EIS). XRD and FTIR studies validate the formation of a complex between the added salt and the polymer matrix. The composition with 60 wt.% of chitosan (CS), 40 wt.% of dextran (DN), and 40 wt.% of magnesium nitrate ($Mg(NO_3)_2$) exhibited the highest conductivity of $\sim 10^{-5}$ S cm^{-1} at ambient temperature.

b0017

Interplay of Attractive and Repulsive Interactions in Tuning Re-entrant Phase Behavior in Charged Colloid

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Silica nanoparticle (anionic, size ~ 16 nm) dispersion undergoes interesting re-entrant phase behavior in presence of polymer or multivalent salt, where the stable one-phase nanoparticle system transforms into aggregated two-phase and then return back to one-phase on monotonic increase in polymer or multivalent salt concentration. The origin of such re-entrant of initial phase in the two cases is entirely different. It is attributed to the multi-valent counter-ion driven charge reversal of the nanoparticles in presence of salt, whereas competition between depletion attraction and polymer-polymer repulsion results in the re-entrant behavior, in case of polymer. Both the systems show a transition from repulsive to attractive to less attractive. We have now examined the modifications in multivalent ion (or polymer) induce re-entrant phase behavior with the help of polymer (or multivalent ions) driven interactions between nanoparticles. It is seen that polymer-induced depletion attraction can suppress the reappearance of the initial phase. Further in contrast to what is observed in nanoparticles on addition of either PEG or ZrCl4, the system undergoes from two-phase to one-phase to two-phase transition at fixed salt concentration and varying PEG concentration. The observed findings are beyond the standard theories of colloidal stability.

b0018

Breakdown of Dynamical Scaling in Confined Geometry: A Real-Time SAXS Study

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Phase-evolution and its kinetics during reactive-dissolution of host-matrix is of immense interest in cementation process. Temporal evolution of structural correlation during hydration-driven gelling across nanoporous spray-dried silica microgranules was investigated. Time-resolved small-angle X-ray scattering (SAXS) experiments quantify the pathway of the pozzolanic gelling extending over around one month. Individuality of the nanoparticles get completely wiped out within a month owing to gelling. The choice of the novel correlated nanostructured silica granules as pozzolans allows unique advantages owing to the special attributes in the scattering profile. SAXS clearly indicated the competitive process arising due to formation and growth of gel at the expense of dissolving nano-silica. The ramified gel evolves non-linearly and follows two-stage sigmoidal dependence. Scaling ansatz breaks down owing to geometrical constraint.

b0019

Unraveling Polyelectrolyte Induced Complex Assembly of Silica Colloids

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Abstract: The anionic silica nanoparticles exhibit intriguing phase behavior, transitioning from a stable phase to turbid phase and further to a milky-opaque phase, with increase in chitosan concentration. In order to understand the structural evolution of the complex colloidal dispersion, small angle X-ray scattering (SAXS) is employed. At low chitosan concentrations, the system forms loose and relaxed aggregated structures with lower volume fraction of silica colloids. In the intermediate concentration regime, an unexpected self-assembled compact structure with high volume fraction of silica colloids are observed. In the high concentration regime, the compact structure loosens, resulting in a decrease in the volume fraction of silica nanoparticles.

b0020

Quantum Insights Into 2D Boron Nitride And Boron Phosphide Biosensors: First Principles Investigation

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Two-dimensional (2D) boron nitride (BN) and boron phosphide (BP) are a lesser utilized materials than other 2D materials in biosensing and their potential in biosensing remains relatively unexplored. In this study, we investigate the biosensing capabilities of 2D BN and BP nanosheets, specifically targeting the ligand such as malarial parasite. From materials science perspective, the interesting physical and chemical properties of the emerging boron nanomaterials are remarkable. By

employing density functional theory, we assess the impact of the malarial parasite ligand adsorption over BN and BP nanosheets and derived the adsorption energy, interaction distance, density of states (DOS) analysis and recovery time. The adsorption energy is -0.059 and -0.0499 eV for BN and BP respectively, with corresponding recovery time 6.0 x 10^{-15} and 5.22 x 10^{-15} sec respectively at 310K temperature. The results presented in this study pave the way for further exploration and development of novel biosensing devices, contributing to the advancement of biosensing technology.

b0021

SANS Investigation of Modification in structure and interactions in Water/AOT/ Dodecane Microemulsion Droplets using tetravalent salts

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The possibility to tailor and control the size, structure, and the macroscopic properties of water-in-oil microemulsions is desirable for a variety of technological applications. In this paper, Small Angle Neutron Scattering (SANS) has been employed to study the formation and various stabilization scenarios of water/AOT/dodecane microemulsion (water confined in oil) droplets. The variation in molar ratio of water to AOT surfactant plays crucial role in tailoring the structure and interactions of the droplets. The complex role of multivalent ions in stabilization of these droplets and modifications of structure and interaction through change of inter-droplet interfacial potential is elucidated using a 2 Yukawa potential.

b0022

Nanocellulose Green Extraction and Fabrication of Electrospun Composite Membrane for Tissue Engineering

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Abstract. Nanocellulose fibers were extracted from invasive species of water hyacinth using a green method of extraction which produced fine nanofibers untreated with acids. The nanofibers were characterized for its morphology, size, chemical structure and crystallinity using TEM, ATR-FTIR, Raman imaging and XRD. Silver nanoparticles decorated nanocellulose were prepared using in-situ synthesis. This nanoparticle attached nanocellulose (AgNP-NC) was used as a filler molecule to impart mechanical strength for poly vinyl alcohol (PVA) nanofiber membrane fabricated using electrospinning. Various concentrations of AgNP-NC were added to PVA solution and electrospinning was done to evaluate the degradation capacity of the membrane in-vitro. The antimicrobial activity of the membranes was also evaluated for its use in tissue engineering.

b0023

Insights Into The Stability Of SARS-CoV-2 Mpro

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Abstract. SARS-CoV-2 Mpro is the key enzyme for viral polyprotein maturation having eleven different cleavage sites in polyprotein. Mpro also known as 3CL protease is a cysteine protease. In order to develop effective measure to prevent the infection and mortality rate, extensive characterization of Mpro stability needs to be studied. There is a dynamic equilibrium of homodimer and monomer which is dependent on its concentration. The activity of dimeric enzyme is more than the monomeric form. SARS-CoV-2 Mpro was recombinantly expressed, purified, and characterized in our lab. In this study, the effect of pH and temperature on Mpro stability was determined using thermal shift assay and fluorescence spectroscopy. Our studies showed that Mpro is stable in a wide pH range and is unstable below pH 4.0 and above pH 9.0.

b0024

Quantum Descriptors under DFT based QSAR study for Oxidative Stress Management of Flavonoids for Inhibition to Linoleic acid for Alzheimer's Disease

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In order to regulate oxidative stress in Alzheimer's disease, this work represents an extensive study on developing quantum chemical descriptors to comprehend inhibition of lipid peroxidation employing flavonoids as anti-oxidant agents. The interactions between inhibitors and the host bio-molecules are extensively investigated calculating electron transfer and energy transfer. The most promising characteristics of flavonoids with linoleic acid have been identified to be energy transfer (ΔE), electron transfer (ΔN), and electronegativity (χ), which can account for around 90% of the inhibition of lipid peroxidation. These novel quantum chemical descriptors are certain to be an outstanding addition to the QSAR expressions used in drug development.

b0025

Expressions for Isothermal Elastic Constants in case of Gay-Berne Potential

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Abstract. One of the central predictions of the KTHNY theory regarding the melting of *2D* solids is that the value of Young's modulus *K(T)* becomes 16π at the melting temperature during the transformation from ordered crystalline phase to a disordered liquid phase. Young's modulus is related to Lame's coefficients which can be calculated from the expressions of isothermal elastic constants. Studies have been done to verify this prediction by considering systems having different types of interaction potentials. In this paper, in order to verify the above prediction, we have derived expressions to calculate the isothermal elastic constants for liquid crystalline (LC) systems whose particles interact via Gay-Berne (GB) pair potential having parameters (3, 5, 2, and 1). Therefore, using these expressions, one can verify the theory's prediction and predict the melting behaviour of LC systems.

b0026

Dwell time distributions for DNA-polymerase motor

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The polymerization of DNA is carried out by a molecular motor, DNA polymerase (DNAP), which is considered as a dual purpose enzyme and is responsible for both the polymerization and exnuclease activity. The motor moves along the track of DNA template step by step and elongates the length of the DNA transcript by successive addition of the nucleotides. The movement of DNAP along the DNA template occurs in a stochastic fashion but on average in a directed manner. In this paper, we consider a minimal model for DNA replication with a purely polymerizing case and with no exonuclease activity. Using master equation approach, we have solved the motion of the DNA polymerase motor and have exactly calculated the dwell time distributions. The nature of such distributions is investigated with different parameters of the model.

b0027

The Effect of hydrophobicity on interfacial water at slightly basic medium for long chain organic molecule -water interface: A MD Simulation Study

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Abstract. Atomistic molecular dynamic simulation has been used to study the behavior of hydroxyl ion (OH^-) at different long chain organic molecule-water interfaces. In the present study, it is observed that the OH^- ion gets accumulated in the long chain alcohol-water interfaces but it does not get accumulated at long chain hydrophobic alkane-water interfaces. The accumulation is found to be guided by the degree of hydrophobicity of the long chain alcohol group along with its capacity to form hydrogen bond with water molecules. Our study also shows that presence of –OH group in long chain alcohol helps to form better alignment of carbon atoms present in the chain. The work also shows the spatial arrangements of bulk water (Hydrogen bond, Tetrahedral order parameter) breaks down near hydrophobic interface but in case of hydrophilic interfaces, the change is minimal.

b0028

Infrared Spectroscopic Studies of Annealed Diglycine Perchlorate Crystal

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Room temperature infrared absorption spectrum of Diglycine perchlorate (DGPCl) was measured and vibrational mode assignments were carried out. The dissociation temperature of this energetic material is reported as ~262°C; thus, to understand the mechanism of dissociation at high temperatures and pre-dissociation phases, different DGPCl crystals were subjected to heat treatment by annealing at various temperatures from 90°C - 210°C. These different annealed samples were allowed to cool and have been studied using infrared spectroscopy at room temperature. It is revealed that the compound shows a melting transition at 103 - 123°C. Above 180°C, the melted phase gradually develops dark brown colour and starts re-crystallizing with modified molecular structure. The phase transition was found to be irreversible upon cooling.

b0029

Nature of Universal Sub-diffusion Crossover in Molecular Glass-Formers

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A crossover from a non-Gaussian to Gaussian sub-diffusion has been observed ubiquitously in various polymeric/molecular glass-formers. We have developed a framework which generalizes the fractional Brownian motion (fBm) model to incorporate

non-Gaussian features by introducing a jump kernel. We illustrate that the non-Gaussian fractional Brownian motion (nGfBm) model accurately characterizes the sub-diffusion crossover. From the solutions of the nGfBm model, we gain insights into the nature of van-Hove self-correlation in non-Gaussian subdiffusive regime, which are found to exhibit exponential tails, providing first such experimental evidence in molecular glass-formers. The validity of the model is supported by comparison with incoherent quasielastic neutron scattering data obtained from several molecular glass-formers.

b0030

Solvent and Temperature Dependent Conformational Changes in Recrystallized Arachidic Acid

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Arachidic acid ($CH_3(CH_2)_{18}COOH$) has widespread use in pharmaceutical and biomedical industries, which demand appropriate solvent selection processes for a wide range of applications. Arachidic acid (AA) is also commonly used for generating multi-dimensional lamellar structures owing to its inherent amphiphilicity. Structural characterization of these crystals, with particular emphasis on the reorientation of their long hydrocarbon chain configuration in response to external stimuli, has not been thoroughly investigated in literature. In this work pure AA has been recrystallized at room temperature from three organic solvents of varying polarity. The effect of each of these solvents on the thermally induced conformational properties of recrystallized AA as compared to pure as-obtained AA, has been studied through Differential Scanning Calorimetry, X-ray diffraction and micro-Raman spectroscopy.

b0031

Ionic Conductivity and the Correlation with Viscosity in Pectin Ionic Liquid Electrolytes

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Biopolymers have received considerable attention for their applications in battery electrolytes due to low cost, easy processability, sustainability, and biodegradability. In this paper, we report the results of pectin-IL electrolytes consisting of pectin and room temperature ionic liquid (IL) 1-n-butyl-3-methylimidazolium hexafluorophosphate ([BMIM][PF_6]). We find that the Nearest-Einstein conductivity (σ_{NE}) decreases with pectin loading. On the other hand, the viscosity increases with pectin loading, indicating the enhancement in the mechanical strength of the electrolyte. Remarkably, we observe an interesting power-law relationship between the σ_{NE} and η such that $\sigma_{NE} \sim \eta^{-1.3}$, an observation that is slightly distinct from the pure IL electrolytes i.e., $\sigma_{NE} \sim \eta^{-1}$. These results offer flexibility in controllably tuning the ionic conductivity and mechanical stability of the IL electrolytes by judiciously choosing the amount of pectin polymer.

b0032

Influences of Cholesterol on Ionic Liquid-Lipid Membrane Interactions

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Here, we report role of cholesterol (CHOL) on the ionic liquid (IL)-biomembrane interaction using surface pressure-area isotherm and Fourier transform infrared (FTIR) spectroscopy techniques. Isotherm results reveal that a few mol% of cholesterol restricts the insertion of long chain imidazolium based IL into the lipid layer formed at the air-water interface. However, this effect is not prominent in case of a relatively shorter chain IL. The FTIR spectrum reveals that addition of cholesterol broadens the main phase transition and shifts it towards the lower temperature. The incorporation of IL into the CHOL-free and CHOL-enriched DPPC membranes induces more gauche defects in both phases, decreasing the transition temperature. Importantly, the presence of CHOL in the membrane weakness the transition strength and enhances fluid phase ordering, highlighting its role in promoting ordering within the DPPC membrane. Our measurements suggested that interaction of IL with biomembrane increases with the increase in the chain length and presence of cholesterol significantly modulates this interaction.

c) Nano-materials

c0001

Facile Synthesis of Luminescent Ultrathin 2D $Ti_3C_2T_x$ MXene Nanosheets

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Since the discovery of MXene, it has drawn tremendous attention from the materials science community for its multifunctional applications in versatile fields such as energy, sensor, catalytic, biomedical applications, etc. This work reports a facile synthesis procedure of 2D $Ti_3C_2T_x$ MXene nanosheets. The phase confirmation and the understanding of the growth mechanism have been done using Rietveld refinement of the powder X-ray diffraction (XRD) data. UV-visible spectroscopy of the $Ti_3C_2T_x$ MXene nanosheets has been measured within the wavelength range of 250-1000 nm. The characteristic peaks near 325 and 783 nm confirm the phase of the $Ti_3C_2T_x$ MXene nanosheets. The band gap of the delaminated $Ti_3C_2T_x$ MXene nanosheets are found 1.99 and 2.01 eV using the Tauc's plot of the UV-visible spectroscopy. The $Ti_3C_2T_x$ MXene nanosheets also show a photoluminescent behaviour. Understanding of the growth mechanism and the structural analysis of the $Ti_3C_2T_x$ MXene nanosheets may be helpful for the realisation of applicational perspectives.

c0002

Hot-injection based synthesis of CdS and CdSe Quantum dots and a comparative study of their properties.

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In recent years, inorganic quantum dots (QDs) have shown promising potentials in various optoelectronic applications, such as light-emitting diodes, solar cells, and photodetectors. Among them, CdS and CdSe QDs showed excellent efficiency towards optoelectronic applications along with stability. Hot injection synthesized QDs show very high stability in ambient conditions as they are capped stable organic ligands. In this work, we synthesized CdS and CdSe QDs using the hot injection method and characterized them with X-ray diffraction (XRD), UV-Vis, and Fluorescence spectroscopy. We also performed a theoretical investigation of the band structure of the bulk CdS and CdSe.

c0003

***In-situ* Solvothermal Synthesis of gCN supported FePc Nanostructure for Visible light assisted Degradation of Methylene Blue**

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We present here a simple and cost-effective solvothermal method for in-situ synthesis of Iron phthalocyanine (FePc) nanostructure supported on graphitic carbon nitride (gCN) sheet. The resulting FePc/gCN nanocomposite displayed promising photocatalytic performances for the degradation of Methylene Blue dye, with removal efficiency of 81% under visible irradiation. A comprehensive understanding of the catalyst's performance along with underlying mechanism has been presented through experimental results and DFT calculations. As predicted by DFT calculations, the existence of a built-in electric field at the interface of FePc/gCN heterostructure suppresses the recombination probabilities of electrons and holes and facilitates efficient charge transport through the gCN architecture. This explains the improved photocatalytic performances of FePc/gCN composite catalyst compared to the pristine components.

c0004

Tailoring Photonic Band Gaps in 1D $CdGeP_2$ Photonic Crystals: A Theoretical Investigation

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In this paper, we have investigated the photonic band structure of 1D CdGeP2 photonic crystals and have additionally examined the impact of filling fraction on band gaps. CdGeP2 is a nonlinear optical material with potential applications in the visible and near-infrared regions. Theoretical calculations using plane wave expansion method demonstrate the ability to engineer and tune band gaps by adjusting the filling fraction. A redshift in band gap is observed with increasing filling fraction. This control over band gaps offers opportunities for customizable spectral properties, making CdGeP2 photonic crystals promising for various photonic devices such as telecommunication devices, IR sensors, biomedical imaging, photonic crystal fiber, photonic hydrogel materials, back reflectors for solar cells etc.

c0005

Effect of Phase Evolution on Structural and Magnetic Properties of $Li_{0.5}Fe_{2.5}O_4$ Annealed at Different Temperatures

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Li0.5Fe2.5O4 was prepared using sol-gel synthesis method using polyvinyl alcohol (PVA) as a chelating agent and then powders were annealed at 700 ° C, 800 ° C and 900 ° C. Rietveld refinement of X-ray diffraction data reveals the ordered phase with $\chi 2$ in permissible range for different annealing temperatures. Average grain size with 435 nm is highest for 900oC annealing temperature and lowest at 291 nm at 800 ° C. Magnetic measurement indicated that the saturation magnetization was found to be maximum for the sample annealed at 800°C.

c0006

Enhancement in Photoluminescence and Photocatalytic Performances of $Mg_3(VO_4)_2$ upon Ce^{3+} Doping

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Ce^{3+} activated $Mg_3(VO_4)_2$ were synthesized by solution combustion route with urea as fuel. Structural, photoluminescence and photocatalytic characteristics of synthesized samples were analyzed by X-ray diffraction (XRD), field-emission scanning electron microscopy (FESEM), photoluminescence (PL) spectroscopy and photocatalytic degradation measurements. The samples are found to have an orthorhombic crystal structure (space group Cmca) of $Mg_3(VO_4)_2$. The crystallite sizes of $Mg_3(VO_4)_2$ and $Mg_{2.99}(VO_4)_2$:$0.01Ce^{3+}$ are found to be 110.92 and 72.22 nm, respectively. The morphology of $Mg_{2.99}(VO_4)_2$:$0.01Ce^{3+}$ exhibits a high degree of agglomeration among fine particles, forming a spherical shape in a three-dimension appearance. The photoluminescence excitation and emission intensities of $Mg_3(VO_4)_2$ are found to enhance upon Ce^{3+} doping. The photocatalytic performance of $Mg_3(VO_4)_2$ for methylene blue (MB) under irradiation from a mercury vapor lamp improves upon Ce^{3+} doping.

c0007

Impact of NH_4ClO_4 and Nitrocellulose on Al-CuO Thermite

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In this research, aluminium-copper oxide (Al-CuO) nanothermites are prepared using a method that involves physical mixing and ultrasonication accompanied by of NH4ClO4, i.e., ammonium perchlorate (AP) and nitrocellulose (NC). This process is a simple, affordable, and conventional technique to create nanocomposites. Differential scanning calorimetry (DSC) is used to study the nanothermite reaction, and it demonstrates that the combination of AP and NC improves the efficiency of combustion and energy release of the aluminum-copper oxide nanothermite.

c0009

Study of Effect of Multi-layer Graphene on the Activation Energy of Al/CuO Nanothermite

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In the present work, Al/CuO nano-thermite reinforced with multi-layer graphene (MLG) sheets is synthesized using physical mixing and ultrasonication techniques, and their activation energy is calculated by the Kissinger fitting method. The phases present in prepared nanothermite are confirmed by X-ray diffraction analysis (XRD). A differential scanning calorimeter (DSC) is used to study the energy release in Al/MLG/CuO nanothermite at different heating rates, and activation energy is calculated using the Kissinger method.

c0010

A Facile Microwave Synthesized MnSeTe Nanosheets for Optoelectronic Application

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Transition metal chalcogenide-based material have grabbed immense interest in various fields like photovoltaic, optoelectronic, and magnetism etc. In the current paper, the Mn based double chalcogenide material is synthesized by the facile microwave technique. Due to the eco-friendly nature of this synthesis method, it is highly appreciated for scale up process also. The structural study reveals the presence of MnSe and $MnTe_2$ phases of the material. Crystallinity of the material gradually decreased with the increase in Se to Te ratio. The alteration in microstructural region is confirmed by the Raman study and it shows the existences different vibrational modes in the sample. With the variation of Se and Te concentration, different MnSeTe nanostructures showed nanosheets like morphology. The optical study showed the blue shift in absorption edge and leads to increase in the optical bandgap. The photo-response study of the material revealed its ohmic behaviour and made it suitable for different optoelectronic application.

c0012

1-Dimensional Polymer Nanostructure from Aromatic Diamine

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In recent years, increasing research interest has focused on the aromatic polymers such as polyaniline (PANI), polypyrrole (PPy), polythiophene etc. due to their conductive nature and good environmental stability which offer wide potential

applications including electrocatalyst, energy storage, electrochromic display, antistatic and anticorrosive materials, sensors. In this regard, one-dimensional (1D) nanostructure morphologies like nanorods, nanowires, nanotubes, nanofibers, nanoneedles and nanobelts are found to be highly desirable owing to their tunable morphology, higher surface area, fast chemical kinetics and rapid doping-dedoping capability. In comparison to monoamine polymers, aromatic diamine polymers offer unique multifunctionality because of one free amino group per repetitive unit on the polymers. In this work, we synthesized 1D polymer nanostructure from poly (*para*-phenylenediamine), which is an aromatic diamine polymer. Potassium persulfate ($K_2S_2O_8$, KPS) was used as oxidant and methyl orange as structure-directing template. These 1D fiber-like polymer nanostructures exhibit rectangular opening and partial crystallinity.

c0013

Fabrication of Self-Assembled $MgFe_2O_4$ Microspheres and Exploration of their Structural, Magnetic and Electrochemical Properties

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Herein, we have synthesized self-assembled $MgFe_2O_4$ microspheres by simple solvothermal technique. Structural and microstructural characterization has been carried out by powder x-ray diffraction (PXRD), field emission scanning electron microscopic (FESEM) and transmission electron microscopic (TEM) techniques. The PXRD pattern shows only peaks for spinel ferrite with $Fd\bar{3}m$ symmetry. The FESEM and TEM micrographs together suggest that the diameter of the spheres lies in the range of 150-300 nm and the microspheres are composed of nanoparticles with crystallite size ~ 48 nm. The microspheres display collective magnetic behavior at room temperature and spin glass like freezing at low temperature. The non-rectangular shape of cyclic voltammetry curves indicates pseudocapacitive behavior of the sample. The sample exhibits maximum specific capacitance of 299 Fg^{-1} at 2 mV/s scan rate and can serve as a supercapacitor.

c0014

Fabrication Of Tungsten Nano-powder Using The "Electric Explosions Of Wires" Method

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Tungsten nano-powder samples with average particle sizes of 47.42nm and 49.03nm were successfully fabricated using tungsten wires (length 3cm, diameter 0.48mm) in an indigenously developed "Electric Explosion of Wires" setup which proves to be economical, portable and time efficient in its production. This setup provides a method of creating nano-sized solid-state particles from bulk solid-state particles in a matter of microseconds, with an intermediary vapour-state. An XRD characterisation was done for the samples, further providing sufficient evidence towards the purity of the sample, so much so that the sample can be used as a standard Tungsten powder sample for future reference. This setup, therefore, overcomes the problems associated with tungsten nano-powder production due to arc discharges related to the surface emission of electrons in Tungsten, by creating a strong pulse (10^5 A/mm2) with a fast pulse rate of 180 A/ns (when charging voltage is 9.5kV).

c0015

Enhanced Luminescence of the Monovalent Sodium (Na^+) codoped $MgAl_2O_4:Eu^{3+}$ Nanostructures

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In the present work, monovalent sodium (Na^+) co-doped $MgAl_2O_4:Eu^{3+}$ photocatalyst was prepared by a combustion method followed by annealing at 1000°C. The doping of trivalent Eu3+ ions into a host $MgAl_2O_4$ with divalent cations leads to luminescence quenching and hence needs charge compensation to control the quenching, which was systematically studied by powder X-ray diffraction (PXRD), diffuse reflectance spectroscopy (DRS), photoluminescence (PL) and X-ray photoelectron spectroscopy (XPS) etc. The PL spectra of doped and co-doped samples exhibit sharp peaks around 580, 592, 611, 628 and 692 nm associated to the $5D_0 \rightarrow 7Fj$ (j = 1–4) transitions of the Eu^{3+} ions, respectively.

c0016

A delve in to the optical properties & stability of citrate capped anisotropic silver nanostructures

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In this work, we systematically investigated the structure-dependent optical properties and stability of citrate-capped anisotropic silver nanostructures synthesized using sonochemical route. The surface plasmon shift from visible to near IR

wavelength, and the control of plasmon damping is monitored by varying capping agent concentration and reaction time. The possibilities of tuning plasmon wavelength to a desired wavelength in the visible to near IR region make it advantageous for label-free sensing applications. The one-pot synthesis approach employed in the study makes the structural tuning facile. The stability analysis is performed by analysing the similarity coefficient of absorption spectra at different time intervals. Physicochemical characterizations are performed using UV-Visible spectroscopy and Transmission Electron Microscopy.

c0017

Effect of Vanadium on Structural and Magnetic Properties of Nano-sized $CoV_xFe_{2-x}O_4$ (x = 0.0 and 0.5) Synthesized by Modified Sol-gel Autocombustion Method

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The $CoV_xFe_{2-x}O_4$ (x = 0.0 and 0.5) nanomaterials were synthesized by modified sol-gel autocombustion method at a relatively lower temperature of 400 ºC (as synthesized products annealed at 550 ºC and 700 ºC).The formations of pure cubic spinel phase products were confirmed by XRD technique. The $CoV_{0.5}Fe_{1.5}O_4$ materials annealed at 550 ºC and 700 ºC exhibits the crystallite size values varying from 30 nm to 40 nm, respectively. There is an overall decrease in the value of lattice parameters as a result of V substitution, e.g. a = 8.349 (5) Å for $CoFe_2O_4$ to 8.320 (2) Å for $CoV_{0.5}Fe_{1.5}O_4$ annealed at 550 ºC, respectively. The Raman studies confirmed the presence of $T_{2g}(3)$, E_g, $T_{2g}(2)$, $T_{2g}(1)$, $A_{1g}(2)$ and $A_{1g}(1)$ modes corresponding to symmetric (stretching and bending) and asymmetric stretching in the spinel lattice structure. The values of M_s decreases from 77.6 emu/g to 66.2 emu/g for $CoFe_2O_4$ and $CoV_{0.5}Fe_{1.5}O_4$ materials annealed at 550 ºC, whereas a decrease from 82.5 emu/g to 68.1 emu/g is noted for the same annealed at 700 ºC, respectively. Also, moderately high values of H_c, i.e. 1229 Oe and 885 Oe, were observed for $CoV_{0.5}Fe_{1.5}O_4$ materials annealed at 550 ºC and 700 ºC, respectively.

c0018

Structural and adhesive properties of Epoxy/GO nanocomposite

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In this work, the effect of the graphene oxide (GO) on structural and thermal properties of epoxy was investigated. Epoxy-GO nanocomposite thin films have been prepared by solution mixing method. The dispersion of graphene oxide in polymer matrix could be improved by pulse sonication method. The binding of GO inside the epoxy matrix was examined through the use of XPS. The XPS analyze the proper binding of GO with epoxy matrix. The T_g of epoxy- graphene oxide is shifted in higher side shows the increase of adhesiveness.

c0019

Moderate Temperature Synthesis of Mn-Based Oxides Using Calcination of Precursors to Check its Potential Applications in NIR (Solar and Color) Pigmentation

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In this work, four different ($MnCl_2.4H_2O$, $MnCO_3$, MnO_2, and $KMnO_4$) precursors were simply calcined at 650ºC/10 hours and examined their calcined products for phase formation of Mn-based oxides and analyzed the suitability of potential application especially for NIR (near-infra red) pigmentation efficiency. Cubic Mn_2O_3 phase materials with space group, *Ia-3* (206) formed for the calcined products of $MnCl_2.4H_2O$ and MnO_2 precursors. However, the purity is differed for the calcined product of $MnCl_2.4H_2O$, for this three weak impurities are noted along with the Mn_2O_3 phase. Mixed phases of Mn_2O_3 and Mn_5O_8 were observed for the calcination of $MnCO_3$ precursor. The resemblance of δ-MnO_2 phase was observed for the calcined product of $KMnO_4$ precursors. While the calcined products of $MnCl_2.4H_2O$, $MnCO_3$, and MnO_2 precursors show the low weight loss of 1.5 – 3.3 %, the calcined $KMnO_4$ precursor shows the weight loss of 22.6 %. The band gap (E_g) calculated from the DRS absorbance data using the Tauc plot reveals E_g = 1.07 eV. The NIR spectrum recorded at 750 – 2500 nm range have the tendency of showing high (45%) NIR reflectance in color NIR region. Nanorod-like morphology was observed for the Mn_2O_3 phase.

c0020

Effective Photocatalytic degradation of non-biodegradable polymer using BiOCl nanostructure

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In this investigation, we achieved successful synthesis and integration of bismuth oxychloride (BiOCl) nanoparticles into LDPE. The nanoparticles exhibited a mesoporous structure with a specific surface area of 22.69 m^2/g exhibiting good photocatalytic properties. FESEM confirmed the homogeneous dispersion and uniform scattering of impregnated BiOCl in the LDPE matrix. Under visible light, the BiOCl nanoparticles efficiently degraded LDPE, generating surface defects. The resulting 86% carbonyl index indicated high degradation due to carbonyl group formation (C=O). EPR analysis also revealed

increased free radical formation. These results demonstrate the potential of BiOCl as an effective photocatalyst for LDPE degradation, offering a promising solution to plastic pollution.

c0021

Organization Of Nematic Liquid Crystalline Phase By In-Situ Synthesis AND Assembly Of Gold Nanocrystal

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In this present article, we report organization of a nematic liquid crystalline phase of MBBA [N-(4 methoxybenzylidene)-4-butylaniline] in presence of Gold nano-crystals (AuNCs) synthesized in-situ within MBBA without using any external reducing and stabilizing agent other than MBBA. AuNCs formed in this growth protocol exhibit assembled structures as observed by Scanning Electron Microscopy (SEM). The most important observation that have emerged through our experiments is organization of the nematic liquid crystalline phase to a completely different ordered phase in MBBA-AuNC composite system which is corroborated well with our findings from Optical Polarization Microscopy (OPM, SEM and Differential Scanning Calorimetry (DSC) study. Combined OPM and SEM observation exhibits formation of leaf-like structures in MBBA-AuNC composite system in contrast to the thread like structure in nematic MBBA. DSC study further indicates pronounced increase in isotropization temperature and enthalpy in composite system compared to pristine sample exhibiting better thermal stability and ordering in composite system.

c0022

Low Temperature Synthesis and Enhanced Magnetic Properties of Nickel Ferrite Nanoparticles Prepared Via Ginger Assisted Green Synthesis Route

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Nickel ferrite nanoparticles were prepared by using sol-gel auto-combustion method with ginger as a green fuel. Single phase formation with cubic spinel structure was verified through X-ray diffraction studies. The crystallite size obtained from Debye-Scherrer's formula was in the range of 14 nm. The lattice constant, crystallite size and other structural parameter were determined from the XRD data. The obtained structural parameters are in good agreement with the literature values. Surface morphology and elemental analysis was performed through scanning electron microscope (SEM). SEM image analysis suggests the formation of spherical grains with some agglomeration. Raman spectrum recorded at room temperature shows five active modes. The saturation magnetization, remanence magnetization and coercivity were measured from M-H hysteresis curve recorded at room temperature using Vibrating Sample Magnetometer (VSM) technique. The saturation magnetization is enhanced whereas coercivity decreases indicating the super-paramagnetic behavior which is suitable for various applications including antibacterial and biomedical.

c0023

Preparation, Composition Analysis, and Electrical Characterisation of Nanoparticulate Pyrochlore $La_2Sn_2O_7$

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This paper elucidates the successful fabrication of nanocrystalline $La_2Sn_2O_7$ ceramic pyrochlore material through a chemical co-precipitation process, followed by conventional sintering. The formation of the pyrochlore phase was verified by Raman spectroscopy and X-ray diffraction, demonstrating the effectiveness of the synthesis method. X-ray photoelectron spectroscopy was employed to gain insights into the sample's surface chemistry and elemental composition and identify its chemical states. Additionally, the electrical characteristics and response of the $La_2Sn_2O_7$ were non-destructively investigated using Electrochemical Impedance Spectroscopy, providing valuable information about its electrical behaviour. The findings of this study contribute to the fundamental understanding of nanocrystalline pyrochlore ceramics and open avenues for their potential applications in various technological domains.

c0024

Blue Emission of Yttrium Doped Zinc Oxide Nanoparticles for Display Technology

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Yttrium (2 mol %) doped ZnO nanoparticles (NPs) were synthesized via hydrothermal process followed by calcination for 1 hrs at 450° C. The calcined sample was characterized using different techniques. The Bragg reflections confirms the formation of hexagonal Wurtzite crystal structure. Irregular shaped NPs are observed on the surface morphology. The energy band gap was tuned to 3.19 eV. The PL emission spectra observed at 325 nm shows the blue emission. The CIE and CCT values confirm that the present synthesized NPs might finds an application in the field of display technology.

c0026

Synthesis and Characterization of Zirconium Oxide and Silver Doped Zirconium Oxide Nanoparticles with their Photocatalytic Performance

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In this research, zirconium oxide (ZrO_2) and silver (Ag) doped ZrO_2 (Ag-ZrO_2) nanoparticles (NPs) were synthesized using the sol-gel autocombustion method and studied their structural, vibrational, and optical properties using various characterization techniques. The crystalline structure and phase purity of these materials were investigated using X-ray diffraction (XRD) analysis. Fourier-transform infrared spectroscopy (FTIR) was employed to analyze the vibrational modes and chemical bonding in the materials. UV-vis spectroscopy was used to study the optical properties of the samples, including bandgap energy and absorbance characteristics. The band gap was found to be 2.56 eV for ZrO_2, and 1.51 eV for Ag-ZrO_2. Photocatalytic performance was assessed by decomposing organic pollutants (MB dye) in the presence of sunlight. The photocatalytic performance of Ag-doped ZrO_2 was investigated to be significantly improved in comparison to pure ZrO2. The % degradation of MB dye with catalyst Ag doped ZrO_2 in the presence of sunlight was found to be 85% in 120 min.

c0027

Insights into the Electronic Structure and Photocatalytic Activity of Double Perovskite Y_2CuMnO_6 Nanoparticles

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This research aims to develop Y_2CuMnO_6 (YCMO) double perovskite with citrate auto combustion method that can be used as a photocatalyst for the degradation of Rhodamine B Dye. XRD and Raman characterization revealed the synthesis of pure-phase YCMO nanoparticles. UV-Vis-NIR analysis estimated a band gap of 2.2 eV, suggesting strong UV and visible region absorption. YCMO nanoparticles resulted in the efficiency of 99%, 93%, and 84% degradation of 5 mg/L, 10 mg/L, and 20 mg/L Rhodamine B dye solution, respectively. Our density functional theory finds that YCMO is a magnetic semiconductor with Cu and Mn in +2 and +4 states, respectively. Thus, our study may promote future research into YCMO double perovskite in the field of excellent photocatalytic potential for environmental application.

c0029

Effect of Film Formation in Polypropylene Graphene Metacomposite

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In this research the effect of incorporation of graphene to polypropylene and the application of heat and pressure to the nanocomposite is studied using dielectric spectroscopy technique and small angle neutron scattering (SANS). Both pellets and films of the polypropylene graphene nanocomposites were made. Graphene was used as it has high electrical conductivity.It is observed that the dielectric constant, dielectric loss, and conductivity are different for the pellets and the films. Negative dielectric constant behavior is observed for both films and pellets. Fractals are observed in both the pellets and films. This research could benefit battery technology and microelectronics.

c0030

Synthesis and Structural and Optical Characterisation of Zn doped Cesium Bismuth Bromide Nanoparticles for Optoelectronic Applications

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Over the past decade, halide perovskites have attracted significant attention due to their remarkable properties, including high quantum yield, tunable band gap, and excellent optoelectronic characteristics. However, challenges related to stability and lead toxicity have hindered their widespread application. As a potential solution, bismuth has been explored as an alternative to lead in halide perovskites and has shown promising outcomes. Property enhancement for optoelectronic applications by the addition of a metal dopant is being investigated here, which could create new non-radiative pathways essential for effective charge separation. The current study is focused on the synthesis, as well as the structural and optical characterization of zinc doped cesium bismuth bromide.

c0031

Electrospun polyvinylidene fluoride mats as a novel platform for dye-doped random lasing

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This article highlights the utilization of electrospun Polyvinylidene fluoride (PVDF) polymer as a system with randomness (scatterers) and rhodamine 6 g (R6G) as the gain medium for random lasers (RLs).By increasing the gain concentration from 1 mM to 3 mM, a transition from amplified spontaneous emission to lasing with coherent feedback is observed. At 3 mM dye concentration, sharp laser peaks (fwhm ≈ 0.2 nm) emerge, superimposed on a broad spontaneous emission background. These findings demonstrate the potential of R6G-doped electrospun PVDF materials as valuable active media for controllable light emission, essential for optical sensing and versatile microlaser devices.

c0032

Influence Of Mn Incorporation On Vibrational Properties And Local Structure Of CeO_2 Nanoparticles

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In the present work, the effect of Mn doping on the local structure of CeO_2 nanoparticles and their vibrational properties have been discussed in the present work. Nanoparticle (NP) formation in pure CeO_2 resulted in modification in bond distances, which is further modified by employing Mn doping of 10 atomic % (at%). However vibrational properties remain unaffected. Variation in atomic distance was observed after incorporating Mn into CeO_2 NPs from absorption measurements. The observed results are correlated and explained on the basis of our previous study which suggested an increase in atomic disorder after doping of Mn into CeO_2. This study may be useful in understanding the structural, vibrational and optical properties of this material as a future work.

c0033

Improved Structural and Thermal Properties of Transition Metal GO/Cu@Fe2O3 Nanocomposite Using Egg Albumin

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Chemical exfoliation and bioinspired methods were used for the first time to synthesize graphene oxide-based transition metal nanocomposite (GO/Cu@Fe_2O_3) using a green synthesis-assisted sol-gel auto-combustion method with the help of egg albumin as naturally capping and reducing agent, which showed eco-friendly, low cost and stability of the fabricated nanocomposite. XRD was performed to know the variation in crystallite size using the Debye Scherrer formula, and microstrain was calculated using the Williamson Hall plot due to doping of Cu in GO/Fe_2O_3 nanocomposite. FTIR results confirmed the functionalized doping of the nanocomposite. Raman analysis showed the purity in the fabrication and proper incorporation of metal ions during fabrication. SEM-EDAX was used to study the surface morphology and elemental composition of the nanocomposite. Further degradation stability was checked at higher temperatures 800℃ of the material using TGA in the nitrogen atmosphere.

c0034

Structural and Electronic Properties of Zigzag Gallium Nitride Nanoribbons

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Nanoribbons, the quasi one-dimensional structures present entirely novel properties as compared to their two-dimensional (2-D) counter parts due to unique electron confinement. Furthermore, the presence of edges provides an easy way to tailor their electronic properties via chemical edge functionalization. In this direction, we have systematically investigated the effect of Br-edge functionalization on the structural and electronic properties of zigzag GaN nanoribbons (ZGaNNR). Present analysis were performed with first-principles calculations using density functional theory (DFT) and the findings were compared with bare and hydrogen functionalized ZGaNNR structures. To comment on the dimensionality effects, nanoribbons having widths Nz = 4, 6, 8 were considered. It is revealed that Br functionalization is mediated via stable chemical bond formation with the edge atoms of the ribbons. Our Stability analysis shows the Br functionalization significantly improves the structural stability even more than that of widely reported H functionalization. However, a small distortion is witnessed in the optimized geometries of Br-functionalized ZGaNNR. H-functionalized ZGaNNR are well known wide band gap semiconductor, however, Br-functionalization leads to significant reduction in the band gap. The obtained band gaps in Br-functionalized ribbons lie between 0.74 eV to 0.19 eV. Overall, our study predicts that Br functionalization of ZGaNNR would be fruitful for the band gap engineering of ZGaNNR for various technological applications.

c0035

Investigation of Structural and Conduction Behavior of $Zn_{1-x}Ga_xO$ Thin Films over a Wide Temperature Range

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In this study, $Zn_{1-x}Ga_xO$ (for x = 0.00 and 0.03) thin films were prepared using sol-gel and spin-coating techniques and the effect of Ga^{3+} ions substitution on structural and dc electrical behavior of ZnO thin films at low temperature varied from 100 – 290 K and voltage scale from 0 – 30 V has been studied using using X-ray diffraction and two-probe conductivity measurements, respectively. The X-ray diffraction results shows that the average crystallite size of doped-ZnO thin film decreases to 16.88 nm from 22.74 nm in case of ZnO thin film. The low temperature electrical study show that electrical resistivity decreases from 2.89×10^2 to 2.29×10^2 Ohm-cm in low temperature range from 290 – 180 K as Ga concentration was increased from 0 to 3%. Furthermore, the presence of thermally activated and hopping type conduction mechanism has been confirmed in Ga-doped thin films up to 100 K. Thus, the ability of Ga-doping to facilitate the conduction process up to 100 K and low activation energy of 0.24 eV in thin films makes it a suitable conductive material for optoelectronic devices.

c0036

Influence Of Cu Dopant On Structural And Photo-luminescence Properties Of ZrO_2 Nanoparticles

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The present study pursued the effect of Cu dopant on ZrO_2 nanoparticles at different doping concentrations (0.01, 0.03 and 0.05 M) using cost-effective co-precipitation technique. X-ray diffraction (XRD) was used to characterize both pure and Cu doped ZrO_2 samples. XRD analysis revealed the monoclinic structure along with some tetragonal trace. No extra peak of impurity phase was observed in all the samples. Further, a slight shifting of XRD peaks towards lower angle indicates that Cu ions were effectively substituted in ZrO_2 lattice. Photoluminescence studies observed that PL emission in the visible region. The emission intensity was found to decrease with dopant indicating the defects induced, oxygen/ionized oxygen vacancies and suppression of electron-hole pairs recombination. Raman spectra also confirmed the monoclinic phase of ZrO_2 with tetragonal traces and absence of impurity peaks as analyzed from XRD analysis.

c0037

Structural, Morphological and Optical Properties of Hydrothermally Synthesized Quasi-Spherical Shaped Copper Vanadate Nanoparticles (CVNP) Towards Environmental Remediation Applications

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The monoclinic Copper Vanadate nanoparticle (CVNP) was synthesized via hydrothermal technique. The structural, morphological, elemental and optical properties of as-prepared CVNP exhibit a monoclinic crystal structure, Quasi-Spherical-like morphology and high photo-response ability. The broad absorption in both UV and Visible regions may boost-up the visible-light-driven photocatalytic activity of CVNP. The photocatalytic performance of as-prepared CVNP was studied by the degradation of organic Rhodamine B (RhB) and Methylene Blue (MB) dye aqueous solutions under visible-light irradiation. The degradation efficiencies of 89% and 93% were achieved for RhB and MB at 60 min of visible-light irradiation owing to its small crystallite size (77 nm) and narrow bandgap (1.88 eV). These excellent characteristics of the as-prepared CVNP strongly suggest that it may serve as a better photocatalyst in the realm of environmental remediation applications for the removal of organic pollutants from wastewater in the near future.

c0038

Flexomagnetodielectric Effect in CuO : SiO_2 Nano-glass Composite System

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Unacceptable leakage currents have imposed severe constraints in downscaling of microelectronic devices. Even while having the same thickness of SiO_2, the "new" high-*k* dielectric material (greater than that of SiO_2 (*k*~3.9)) can provide a substantially greater physical thickness (defined as equivalent oxide thickness (EOT)) to solve the technical problem of direct tunneling leakage current. A composite system of SiO_2 implanted with nanoparticles of CuO 0.5 mol % prepared was via sol-gel route calcination at 700°C & above. The superparamagnetic nanoparticles are spherical, nearly uniform, and homogeneously dispersed in the matrix, a rapid decline in ε' at low temperatures is attributed to the presence of thermally activated relaxation process. Relaxation time (τ) follows Arrhenius law and activation energy E_a decreases with increasing magnetic field. The observed near room temperature enhanced dielectric constant (nearly 2.3 times over the SiO_2) and a negative magnetodielectric effect (14%) attributed to the flexomagnetoelectric effect.

c0039

Enhanced nonlinear characteristics of polymer-perovskite hybrid (PVA/CMC/$LaAlO_3$) fabricated via solution casting process for optical limiting applications

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Hybrids of polymer-perovskite are fascinating materials that are highly suited for electric and optoelectronic application since they possess enhanced physical and chemical properties. In the current work, polymer nanocomposite (PNCs) films based on polymer blend matrices (i.e) carboxy methyl cellulose (CMC)/Polyvinyl alcohol (PVA) in 30:70 wt% ratio integrated with sol gel synthesized ceramic LaAlO3 nanoparticles (NPs) were prepared by the solution casting technique. The chemical compositions and the degree of crystallinity were investigated by FTIR and XRD analysis respectively, to study the impact of nanoparticles on the polymer blend structure and the complexation within the functional groups of the hybrid PVA/CMC system. Morphology analysis (SEM) reveals the surface roughness and variation with the inclusion of nanoparticle content. The UV-Vis spectrophotometer brings out the optical characteristics of PVA/CMC /LaAlO3 PNCs. Also, as a result of loading nanoparticles the optical gap of PVA/CMC blend is boasted. The third order optical nonlinearity of LaAlO3 incorporated PVA/CMC blend was determined by standard Z scan technique using 532nm CW DPSS and Nano pulsed Nd:YAG laser. The results confirm that PVA/CMC/LaAlO3 thin films would prove to be promising candidates as optical limiters in safeguarding optical components from high intense laser pulses. Further lower onset optical limiting threshold under pulsed laser excitation of PVA/CMC/LaAlO3 NPs (1.14 X 1012 Wm-2) in comparison to pure LaAlO3 NPs (4.42 X 1012 Wm-2) clearly confirms that incorporating LaAlO3 NPs within the polymer matrix could yield efficient energy absorbing optical limiters.

c0042

Charge Transfer Mediated Third-Order Nonlinear Optical Response in $CsPbBr_3$-Single-Wall-Cabon Nanotube Hybrid

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The realization of the large optical nonlinearities at low fluence holds great promise in fundamental studies and photonic applications. In this letter, we experimentally demonstrate large reverse saturable absorption (RSA) and self-focusing in the $CsPbBr_3$-single-wall carbon nanotube (SWCNT) hybrid. Strikingly, we perceive that a higher excited state absorption cross-section exceeds the ground state absorption cross-section, which suggests that they can be employed as passive optical limiters. The observed RSA coefficient and nonlinear refraction are discussed in the framework of an efficient charge transfer between the $CsPbBr_3$ nanocrystal (NCs) and SWCNT. Further, steady-state photoluminescence (PL), time-resolved PL, and transient absorption measurements corroborate our idea of charge transfer from $CSPbBr_3$ to SWCNT. Moreover, we also demonstrate a liquid cell-based optical limiter device with performance parameters such as onset threshold (F_{ON}) of 0.01 GW/cm^2, and optical limiting threshold (F_{OL}) of 0.03 GW/cm^2, which are on par with several other benchmark optical limiters.

c0043

Structural, Optical and Dielectric Properties of LaCr1-xCoxO3 (x = 0.0, 0.1, 0.3, 0.5) Nanoparticles

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In this work, we have synthesized LaCr1-xCoxO3 (x = 0.0, 0.1, 0.3, 0.5) NPs using the sol-gel method. The synthesized samples has been thoroughly characterized using various techniques including are XRD, SEM-EDX, UV- visible absorption spectroscopy and LCR meter measurements. The XRD analysis revealed that the sample of possesses a pure single- phase in orthorhombic structural phase belonging to Pnma space group. SEM micrographs and EDX spectra of the LaCrO3 and LaCr0.5Co0.5O3 samples depict the particles are easily observable to the composed of clusters formed by these tiny particles and the display of presence of peaks associated with the constituent elements (La, Cr, Co, O). UV-visible spectroscopy has been employed to determine the band gap value for the samples of NPs, using Tauc's relation. The dielectric properties of the samples were investigated through the dielectric constant and loss measurements, which showed a decreasewith increasing in frequency and the a.c.conductivity of the sample exhibited an increase with higher frequencies.

c0045

Structure Correlated Magnetic Properties of Sr Doped $NiFe_2O_4$ Nanoparticles

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Nanoparticles of Sr-doped $NiFe_2O_4$ samples, synthesized by auto combustion method, were studied for their structure correlated magnetic properties. The samples were characterized by X-ray diffraction, Raman spectroscopy and a vibrational sample magnetometer. A cubic spinel-type structure for each sample, with an average crystallite size in the range of 13–43.5 nm, was confirmed by the XRD. Sr doping resulted in increased crystal lattice parameters due to larger Sr^{2+} ion radius. Five active phonon modes of spinel phase are observed in Raman spectra. The cations at the tetrahedral and octahedral sites get rearranged due to the Sr doping causing an increase in magnetic properties of $NiFe_2O_4$.

c0046

Synthesis of Bimetallic Ni-Co MOF for Photocatalysis Application

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Bimetal metal organic framework (MOF), the Ni-Co-MOF was synthesized by a one-pot solvothermal method with nickel and cobalt as metal ions and terephthalic acid as organic ligand. The crystal structure was confirmed using X-ray diffraction. More precisely the structure of this bimetallic MOF was determined using Raman scattering experiments. Compositional analysis by X-ray photoelectron spectroscopy showed that the presence of Ni, Co, Cand O. The band gap of the Ni-Co-MOF was found to be 2.3 eV. The band gap is found to be low and it serve as an active photocatalyst in photocatalysis process. It has been tested for the photodegradation of methylene blue (MB) dye under UV light irradiation that resulted in 26.69% efficiency in degrading the MB dye.

c0047

Room-Temperature Xylene Detection Using WSe_2/MWCNT Composite

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In this brief article, we are reporting a xylene sensitive and selective chemeresistive composite sensor based on WSe_2 (p-type)/MWCNT (p-type) heterojunctions working at room temperature. In comparison to pristine WSe_2, composite sensor performsway better by obtaining 1.15 times higher response (0.92%) and full recovery. In addition, the composite-based sensor has a cleanand consistent response throughout a wide range of xylene concentrations, as well as a highly selective character towards xylene when compared to other analytes. Lowest limit of detection for composite sensor has been calculated to be 12.82 ppm. As a result,our study opens the door for composite-based (p-p type) heterojunctions to be used in real-world applications for monitoring hazardous gases such as xylene.

c0048

Study of Electrical Properties of $La_{0.7}Sr_{0.3}MnO_3$- Polyvinylidene Fluoride Hybrid Flexible Film for Wearable Electronic Device

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The field of flexible magnetoelectric composite film attracts researchers due to the preparation of wearable electronic devices. Quest of significant composition to prepare effective magnetoelectric composite, the Polyvinylidene fluoride based inorganic-organic hybrid composite flexible film attains research interest. In this point of view we are also interested to prepare composite flexible film with the composition of in-organic $La_{0.7}Sr_{0.3}MnO_3$ and organic Polyvinylidene fluoride, with weighted ratio 50:50. In this context, we have investigated AC electrical properties of 0.5 $La_{0.7}Sr_{0.3}MnO_3$ - 0.5 Polyvinylidene fluoride nanocomposite flexible film with the variation of applied magnetic field at room temperature. The AC electrical properties of the composite reveal a change in impedance when a magnetic field is applied, due to the magnetostriction property of the piezo-magnetic phase of the composite. As the magnetic domains are align along the direction applied magnetic field, leads increasing of mobility of charge carriers. The maximum value of the change is found to be ~ 0.8% at constant frequency of 1200 Hz and applied magnetic field of 1200 Oe.

c0049

Magneto-Impedance of Zn0.5Ni0.5Fe2O4 – Polyvinylidene Fluoride Hybrid Nanocomposite Flexible Film

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Due to the increasing interest at present time in the field of wearable electronics, the flexible composite film leads intense research interest for the core researchers. In this context, we have presented the magneto-impedance studies of $0.5Zn_{0.5}Ni_{0.5}Fe_2O_4$ - 0.5polyvinylidene fluoride nanocomposite flexible film prepared through low temperature "pyrophoric reaction process" succeeded by casting method. The magneto-impedance properties of the composite flexible film have been studied employing magnetic field depending impedance spectroscopy technique. The value of impedance is found to decrease in nature with increasing strength applied magnetic field, as a cause of high interfacial polarization at the low field strength of the granular like composite. Moreover, with the increasing strength of the applied magnetic field, the value of impedance also found to be decreased in nature or the increasing value of magneto-impedance, attributing the magnetostriction property, domain alignment of the piezo-magnetic phase and transfer of stress to the piezoelectric phase from the magnetic phase of the composites. The maximum value of the magneto-impedance is found to be ~5.3 % at a frequency of 2200 Hz, having applied magnetic field of 1800 Oe.

c0050

Enhanced Humidity Sensing Behavior of Sol-Gel Derived ZnO-C65 Heterostructure Thin Films

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Humidity sensing characteristics of conducting carbon C65 modified ZnO heterostructure films are reported. ZnO and ZnO-C65 heterostructure films are processed using sol-gel technique by adding different concentration of C65 carbon. Crystalline and morphological features of the samples are examined by X-ray diffraction and scanning electron microscopy studies. Change in the morphology of the ZnO particles is observed upon addition of C65 carbon. Humidity sensing studies on ZnO-

C65 heterostructure films have shown enhanced sensitivity factors than pure ZnO films. The results are attributed to the formation of heterostructures of conducting C65-semiconducting ZnO, and nanostructured morphological changes.

c0052

Synthesis And Spectral Investigation Of Sm3+ Doped KZr2(PO4)3 Phosphor

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The solution combustion approach with urea as fuel is used to successfully synthesize Sm^{3+} doped $KZr_2(PO_4)_3$ phosphor The XRD data support the synthesis of single-phase powders, with crystallize sizes of 38 *nm* for the undoped sample and 43 *nm* for the Sm^{3+} doped sample. The Photoluminescence emission spectra used to study emission spectra of the phosphor shows four traditional bands of the Sm^{3+} ion. The concentration quenching is observed at concentration more than1.5 mol. %. The band gap of the sample was obtained by using DRS spectra. The bandgap value for the optimal sample turned out to be 4.5 eV.

c0053

Metal-Organic Frameworks based Triboelectric nanogenerator as a self-powered tactile sensor

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Self-powered sensors are gaining attention nowadays because of their flexibility in various applications. Wearable technology demands self-powered sensors drastically. Self-powered sensors can be easily constructed using a Triboelectric nanogenerator, which works based on the principle of contact electrification and electrostatic induction. TENG converts mechanical energy into electrical energy. Based on the difference in charge affinity, a triboelectric series is set up, which demands novel materials. Metal-Organic Frameworks are the novel materials getting added to this series. This paper discusses the triboelectric property of ZIF-8, a sub-class of MOF, and it can be employed as a self-powered tactile sensor. The open circuit voltage obtained for the Z-TENG is 75 V, and the short circuit current of 12 µA. The device is used to power a display based on the touching activity of a human hand.

c0055

Understanding the Effect of Variation in Co to Ni Ratio on the Meso-structure and Evolved Vacancy Defects in $NiCo_2O_4$ Nanowires

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Tailoring morphology and defect architecture plays a crucial role to improve the performance of Transition Metal Oxide (TMO) based heterogeneous catalyst for sustainable energy applications. Adopting similar approach, defect-rich, one dimensional $NiCo_2O_4$ (NCO) nanowires with significantly high surface area and porous architecture were synthesized via a simple solvothermal method. Variation in the ratio of Co to Ni content was chosen as the strategy to engineer the defects in these nanowires. All the calcined NCO samples were observed to be phase pure from Powder XRD study. FE-SEM and TEM measurements confirmed the nanowire morphology and homogeneous elemental distribution along a single nanowire. N_2 adsorption-desorption studies showed substantially high surface area and mesoporous architecture of the nanowires. Positron lifetime measurement indicated creation of Co vacancies or Ni_{Co} antisite defect in Co-deficient NCO samples, whereas, preferential formation of larger vacancy clusters at the surface was observed in Co-excess samples. This study will provide further insights for designing transition metal oxide based multifunctional materials with desired defect and surface characteristics.

c0057

Green Synthesis of Mixed Ni-Zn Spinel Ferrite Nanoparticles and Study of Structural, Optical, and Magnetic Properties

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The important structural and magnetic properties are important parameters for biomedical, photocatalytic and other applications. In the present work, mixed Nickel-Zinc ($Ni_{0.7}Zn_{0.3}Fe_2O_4$) nanoparticles were synthesized by novel green synthesis method assisted by aqueous extract of black pepper. These nanoparticles were characterized by various techniques such as X-ray diffraction (XRD), Infrared spectroscopy, Raman spectroscopy, UV-Visible Spectroscopy (UV-Vis's) and Vibrating sample magnetometer (VSM), Uv-Visible Spectroscopy (Uv-vis). The results of XRD data revealed the formation

of single-phase cubic spinel structure with average crystallite size of the order of 19 nm. Fourier Transform Infrared (FTIR) spectrum show two main absorption bands near 400 cm^{-1} and 600 cm^{-1} indicative of cubic spinel structure. Raman spectrum recorded at room temperature shows five active modes. The hysteresis curve represents typical superparamagnetic behavior. The band gap obtained from Tauc plot is of the order of 1.88eV. The obtained structural, morphological, magnetic and optical data may be useful for magnetic hyperthermia applications.

c0058

Tunable Emission of Quantum LEDs

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Quantum dot (QD) based tunable light emitting diode (Q-LED) is the goal for next-generation display systems to meet the tailored requirement of advanced applications, such as cell phones, flexible technologies, and large area display technologies with ultrahigh-definition etc. The tunability of emission from Q-LEDs highly depends on the nature of the quantum efficiency and the respective size of quantum dots. Here, we demonstrate a tunable emission from Gallium Arsenide (GaAs) PN-junction in the presence of different types of QDs due to the recombination of charge carriers confined at the bottom of the QDs. Thus, the potential tunability of emission from quantum dots-based GaAs Q-LEDs motivates the development of future-generation reconfigurable Q-LEDs emissions for highly efficient display technologies.

c0059

Synthesis and characterization of $La_2Zr_2O_7$ and $Nd_2Zr_2O_7$ pyrochlores

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Pyrochlore material are interesting candidates studied for various applications. In this work, two pyrochlore materials such as $La_2Zr_2O_7$ (LZO) and $Nd_2Zr_2O_7$ (NZO) were synthesized via co-precipitation method. They were characterized using XRD, UV-Vis-NIR and XPS spectroscopy. The XRD shows the space group Fd-3m structure in both LZO and NZO. The crystallite size of LZO ranged between 11.8 nm and 14.9 nm, while the same for NZO varied from 10.1 nm to 20.2 nm as calculated using W-H method and Scherrer formula. The chemical composition and the oxidation states of individual elements were studied using XPS.UV-VIS-NIR spectroscopy analysis revealed that LZO has a band gap of 5.4 eV, while NZO has a slightly lower band gap, 5.2 eV.

c0060

Fe_2O_3-MoS_2 Nanocomposite for Enhanced Electrocatalytic Hydrogen Generation

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In pursuance to achieve green future, electrochemical water splitting can be potential technology to address the global need to replace the polluting fossil fuels. In order to search non precious and non noble metal based electrocatalysts we successfully synthesized Fe_2O_3-MoS_2 via two step facile synthesis route. Fe_2O_3-MoS_2 exhibits significant lower overpotential, 202 mV, to drive 10 mA cm^{-2} current density and the value is superior to the individual components, Fe_2O_3 and MoS_2. The low charge transfer resistance 13.9 Ω signifies the faster charge transfer at the electrolyte-catalyst-interface facilitating HER performance. The sample also shows good stability and durability under the acidic medium. The higher value (10.3 $mFcm^{-2}$) of electrocatalytic double layer capacitance C_{dl} corresponding to Fe_2O_3-MoS_2 composite further confirms the ample availability of electrocatalytic active sites. The study establishes a successful TMO –TMD composite as a potential candidate for HER performance in acidic medium and opens up new opportunities for finding proper electrocatalyst towards 'green hydrogen'.

c0061

Electrochemical Studies of Silver doped Nanoceria

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Abstarct: In this work, CeO2: Ag (12 mol%) NPs were synthesized utilizing a solution combustion approach with Aloe vera extract as a reducing agent. The collected NPs were characterized using standard methods. Braggs reflections reveal the formation of a single-phase Cubic structure of CeO2: Ag NPs. Both Scherrer's equation and the W-H plot are used to determine crystal size. Ce, O, and Ag were indeed present, according to the EDAX pattern. Wood and Tauc's calculations revealed that the direct energy band is 2.9 eV. The functional groups were present, according to FTIR analysis. Furthermore, electrochemical investigation reveals that synthesized NPs have the largest specific capacitance at the slowest scan speeds. According to CV, GCD, and EIS, Ag-doped CeO_2 NPs have potential uses in energy storage devices such as supercapacitors.

c0064

Eu^{3+} Assisted Luminescence in $SrWO_4$:Eu^{3+} Phosphors

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In the luminescence world phosphors doped with rare earth have covered large percentage. In the addition of ongoing research our work centred at luminescent materials which is Eu^{3+} doped $SrWO_4$ phosphors. This work, $SrWO_4$ and Eu^{3+} doped $SrWO_4$ were synthesised via co-precipitation method. X-ray diffraction tells us about the tetragonal structure of sample and the samples belong to the space group of I41/a. The PL of all the phosphors were monitored. The Eu^{3+} doped phosphors also exhibit colour emission proving its utility in the field of lighting application. Thus, our phosphor study shows we can use it in lighting application.

c0066

Investigation on Optical and Magnetic Properties of Hydrothermally Synthesized La Ion Doped Mg-Zn Nano-ferrite

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In this article, the optical and magnetic behaviour was studied for varying the concentration of Lanthanum (x= 0, 0.25, 0.5) ion in Mg-Zn ferrite prepared using the convenient hydrothermal method. The nanomaterials exhibited spinel ferrite structure with *Fd3m* space group. There was an increase in crystallite size with a higher La concentration. An almost spherical, homogeneous, and agglomerated nanoparticles with all the constituent elements were detected through FESEM and EDX techniques. The energy band gap was found to decrease with an increase in La concentration. The dopant concentration also affected the magnetic properties with a decrease in saturation magnetization and enhanced coercivity.

c0067

$KMnO_4$ and Ascorbic Acid Sensing Study using Ce^{3+} and Tb^{3+} Doped $NaGdF_4$ Core and Core shell Monodispersed Nanoparticles

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A series of Ce^{3+} and Tb^{3+} doped $NaGdF_4$ core and core@shell monodispersed nanoparticles with different doping of Ce^{3+} and Tb^{3+} in $NaGdF_4$ core and core@shell nanoparticles $NaGdF_4$:Ce20%@$NaGdF_4$:Tb5% (C-20Ce@S-5Tb) and $NaGdF_4$:Tb5%@$NaGdF_4$:Ce20% (C-5Tb@S-20Ce) NPs have been synthesized using thermolysis method. Ce^{3+} shows the absorption peak in 250-260 nm, Gd^{3+} shows the absorption peaks at 278 and 310 nm and Tb^{3+} shows the absorption peaks at 350 and 378 nm. In Ce-Tb system, there is an energy transfer from Ce^{3+} to Tb^{3+} and thus, a significant enhancement in luminescence intensity (488 and 545 nm) is observed. This is due to overlapping of absorption peak from Tb^{3+} with emission peak from Ce^{3+}. The energy transfer from Ce^{3+} to Tb^{3+} is significantly improved in core@shell nanoparticles as compared to that of core nanoparticles. The $KMnO_4$/ascorbic acid sensing was performed in all the silica coated core and core-shell NPs. It was found that the Ce^{3+} in the surface/shell of C-5Tb@S-20Ce sample was more exposed to $KMnO_4$/ascorbic acid, so it is most sensitive, cheapest material for the sensing behavior.

c0070

Facile construction of $FeWO_4$/MWCNT composite to effectively degrade the textile effluent and refractory pharmaceutical pollutants under white light

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An effective hydrothermal technique was developed to prepare ferrous tungstate/Multi-walled carbon nanotubes ($FeWO_4$/MWCNT) composite for photocatalytic activity. The structural, optical, morphological and elemental composition of the prepared composites were carried out by X-Ray Diffraction (XRD), UV–vis Diffuse Reflectance Spectroscopy (UV-DRS), Photoluminescence Spectroscopy (PL), Scanning Electron Microscopy (SEM), and Energy Dispersive X-Ray Spectroscopy (EDX) respectively. The photocatalytic degradation performance of the Methylene Blue (MB) and tetracycline (TC) decomposed in the presence of composite under white light irradiation. The inclusion of MWCNT in FWO exhibits better photocatalytic degradation efficiency than pristine FWO, and a reason with an explanation is given below.

c0072

Focused Ion Beam Milling Based Nano-patterning: Towards the Nano-photonic Applications

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Focused ion beam (FIB) technique has been emerging, in recent times, as one of the most efficient and powerful tools for nanofabrication with its own merits, including rapid, site-specific, mask-less (single-step) processing and suitable for unpolished surfaces. In this work, we exploit the potential of this technique towards nano-photonic application. A high-index and less expensive Si wafer, the backbone of the semiconductor industry, is used for this purpose. An advanced Raith Nanolithography module attached to the basic FIB unit facilitates the nano-lithography functionality with nanometer scale accuracy. Cone-shaped Ga ion beam milled nano-etch-pits were created by controlled FIB milling over an area of 0.2 by 0.2

mm. The pit dimensions were controlled by the FIB milling parameters. 2D arrays of nano-etch pit patterns with various periodicities were prepared, and their reflectance spectra were measured. It was found that the patterns reflected various vibrant colors depending on the periodicity, meaning that by controlling one of the pattern parameters, it was possible to control the reflected wavelength. The multiple resonances of the 2D lattice of the nano-etchpits are attributed to the color filtering properties of the Si meta-surface.

c0073

Synthesis and Characterization of Halloysite Nanotubes (HNTs) Adorned Chicken Eggshell Powder as Low-cost Adsorbent Towards Hg(II) Removal

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Mercury is a well-known heavy metal pollutant of global importance, as it is highly toxic to humans, animals and plants. The present work aims at the preparation and characterization of chicken eggshell based green adsorbent (BESHN) for the effective adsorption of Hg(II) from water. where a simple ball milling method was adopted. The Environmental Protection Agency has declared eggshell waste as the 15th largest food industry pollutant. The highly porous nature of chicken eggshell powder (CESP) and the cation exchange capacity of HNTs are considered as adsorbents for the removal of heavy metals. The prepared BESHN nanocomposite was subjected to XRD, FTIR, SEM and EDX studies which strongly confirm the adornment of HNTs at the surface of CESP. The adsorption efficiency of CESP and BESHN towards Hg(II) was found to be 74% and 82%, respectively. The addition of HNTs into the CESP matrix could adsorb more Hg(II) and thereby enhance the removal performance. Hence these results ensure that the prepared BESHN adsorbent may be a budding choice for the removal of mercury in the realm of wastewater treatment.

c0074

Investigation of Structural and Optical Properties of Ni Substituted SmFeO3 Nanoparticles

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In this study, nanocrystalline powder samples of $SmFe_{1-x}Ni_xO_3$ ($0 \leq x \leq 0.3$) have been prepared via sol-gel citrate route. The structural phase purity of the synthesized samples is corroborated by Rietveld refined XRD patterns. Average crystallite size and crystallographic strain introduced on account of Ni substitution were calculated using the Williamson-Hall analysis. FTIR spectra exhibit two strong absorption bands around 554 cm^{-1} and 416 cm^{-1} linked to the metal oxide (Fe/Ni-O) stretching and O-Fe-O deformation mode of vibrations respectively. UV-visible spectroscopy manifests a remarkable reduction in the optical energy band gap on increasing Ni content. It is observed that with Ni substitution, crystallographic strain increases and Urbach energy follows the similar trend.

c0075

Study of Annealing Effect on the Structural and Optical Properties of Cobalt Oxide Nanoparticles Synthesized by Hydrothermal Method.

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Cobalt oxide nanoparticles have potential applications in energy storage devices. This study investigated the structural and optical properties of Co_3O_4 nanoparticles synthesized by hydrothermal method. The as-prepared and annealed samples were observed for their structural and optical properties. The structural analysis and micro-strain effects of Co_3O_4 nanoparticles with cubic spinel structure were carried out through XRD. The crystallite size of as-prepared and annealed samples were around 27 nm and 29 nm, respectively. Raman spectrum showed the lattice vibrations of both oxidation states of cobalt oxide nanoparticles. The optical studies were done using the absorption spectrum and photoluminescence spectroscopy. Two direct band gaps were observed in as-prepared samples, which got red-shifted on annealing due to size effects. The charge transfer process in two oxidation states of cobalt oxide could be identified from these bandgaps. Emission peaks in the photoluminescence spectrum of samples are due to the recombination of free-excitons and point defects in the crystal lattice.

c0076

Emission Tuning in Eu^{3+} Doped Calcium Magnesium Silicate Phosphor via Annealing Temperature

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Eu^{3+} doped calcium magnesium silicate (CMS: Eu^{3+}) phosphors show emission in the red region suitable for the red components in w-LEDS and bioimaging. Tuning of emission properties, decay time and color chromaticity of CMS: Eu^{3+} via changing the annealing temperature is employed in the present study. For that CMS: Eu^{3+} was synthesized via sol-gel route at a pH of 2 and annealed at 800˚C and 1200˚C separately. The morphology analysis reveals the particle formation at 1200˚C. A combination of diopside ($CaMgSi_2O_6$), merwinite ($Ca_3MgSi_2O_8$) and monticellite ($Ca_{0.88}Mg_{1.12}SiO_4$) phases of the monoclinic crystal structure are identified with XRD analysis irrespective of annealing temperature. The photoluminescence studies confirm the increase in the intensity and splitting, lifetime analysis reveals the increase in the decay time and color chromaticity

studies show the tuning of the color to a redder region of the CMS: Eu^{3+} with the increase in annealing temperature. The enhanced photoluminescence properties with decay time and color chromaticity suggest the proper site occupancy of Eu^{3+} with better charge compensation in calcium magnesium silicate (CMS) host with increased annealing temperature.

c0077

Degradation and Molecular level analysis of UV Light induced photodegradation of Rh 6G by g-C_3N_4

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The photodegradation of Rh 6G dye utilizing g-C_3N_4 photocatalyst under UV light has been investigated and reported in this paper. The straightforward pyrolysis process was used to prepare the photocatalyst, g-C_3N_4. XRD, UV-Vis spectroscopy, XPS, SEM, and EDS were used to analyze the structure, optical characteristics, elemental composition, morphology and composition of elements in g-C_3N_4, respectively. Using g-C_3N_4 as photocatalyst, the Rh 6G dye was degraded up to 99.6% in 300 mins under UV light. The photocatalysis process was monitored utilizing UV-Vis absorption spectroscopy. To have a molecular level understanding the process, the active radicals participated in the degradation process was investigated using appropriate scavenger molecules.

c0078

Synthesis and Characterization of 2H-MoS_2 Prepared by Sol-Gel Process

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Two-dimensional (2D) nanostructured materials are extensively used in photonics, optoelectronics, catalysis due to its excellent physical and chemical properties such as quantum confinement, high absorption coefficient, high surface to volume ratio, tunable band gap etc., Molybdenum di-sulfide (MoS_2) is an important 2D nanomaterial, in which hexagonal form shows interesting properties. Herein, 2H-MoS_2 was successfully synthesized by sol-gel process using different sulfur sources as thioacetamide (TA) and thiourea (TU). Effect of different sulfur sources in MoS_2 is investigated. X-Ray Diffraction studies of MoS_2–TA and MoS_2 –TU reveal that the hexagonal (2H) structures have an average crystallite size of 15 nm & 22 nm respectively. The hexagonal (2H) phase is confirmed by E^1_{2g} (in-plane) and A_{1g} (out-of-plane) phonon modes of Raman spectrum. The oxidation states of MoS_2 are observed by using core level XPS spectrum of molybdenum (Mo 3d) and sulfur (S 2p).

c0079

Lithium Extraction from Simulated Wastewater using Capacitive Deionization

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To extract the valuable elements from wastewater, capacitive deionization (CDI) has emerged as energy-efficient method among other desalination methods. Herein, we report the extraction of lithium from simulated aqueous lithium chloride solution by CDI technique. The lithium extraction was carried out using hybrid CDI (HCDI). The HCDI comprised of manganese oxide decorated on solar reduced graphene oxide (SRGO-MnO_2) as a lithium selective electrode material, and SRGO along with anion-exchange membrane on respective electrodes. The SRGO-MnO_2 electrode served as lithium selective electrode, and SRGO with anion-exchange membrane served the purpose of anion capture. The morphology of the as-synthesized electrode materials was characterized by scanning electron microscopy. The elemental analysis was performed by energy dispersive x-ray spectroscopy. Moreover, the chare storage behavior and specific capacitance of the as-synthesized materials were estimated by cyclic voltammetry, and galvanostatic charge-discharge techniques. The specific capacitance of SRGO-MnO_2 (185.25 F/g) was higher as compared to SRGO (52.77 F/g) and MnO_2 (35.55 F/g), at a scan rate of 10 mV/s. Therefore, it is anticipated that MnO_2 served as pseudocapacitive/faradaic component, which helped to increase the specific capacitance as well as salt adsorption capacity during electrosorption experiments. The salt adsorption capacity was marginally higher for HCDI (54.44 mg/g), due to the synergistic effect of cation-specific adsorption of MnO_2 particles on the surface of SRGO, high conductivity of SRGO, and high specific capacitance of SRGO-MnO_2 composite.

c0080

Impact behaviour of UHMWPE/MXene Nano composite

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This research focuses on the fabrication of UHMWPE/MXene nanocomposites via a solvent mixing approach, subsequently followed by compression molding. The structural properties of the resulting composites were analyzed using X-ray diffraction (XRD), confirming their composition and arrangement. Additionally, the thermal stability of the nanocomposites was assessed through Thermogravimetric Analysis (TGA-DTA), providing valuable insights into their thermal behavior. Moreover, the impact studies conducted on these nanocomposites shed light on their mechanical performance and potential applications. The combination of UHMWPE with MXene represents a promising avenue for developing advanced materials with enhanced properties and performance for various engineering applications.

c0081

Application of TiO2 nanorods in perovskite solar cells

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Hole transport material-free carbon electrode-based perovskite solar cells (C-PSCs) are one of the hopeful solutions for the availability of PSCs in the market. However, there is still some potential to increase the carrier collection in this cutting-edge system. In that respect, Strontium (Sr^{2+}), an effective alkaline earth metal ion has been used as a dopant in the rutile TiO_2 NRs. The rutile TiO2 nanorods (NRs) with Sr^{2+} dopant was synthesized through the solvothermal route. The phase and morphological confirmations of the synthesized samples were done by PXRD and FE-SEM analysis, respectively. The performance of the fabricated solar cells was studied in depth through J-V measurement. It was found that the device with optimized wt% of Sr dopant attains PCE of 11.1% with Jsc of 21.028 mA/cm^2.

c0082

Study of Luminescence Properties of Ce^{3+} Doped β-$Ca_3(PO_4)_2$ Phosphor via Modulation of Annealing Temperature

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The present study explores the correlation of structure and luminescence properties of Ce^{3+} doped $Ca_3(PO_4)_2$ phosphor materials with the annealing temperature. The $Ca_3(PO_4)_2$ and $Ca_3(PO_4)_2$:Ce^{3+} are synthesized using the conventional solid-state reaction method at 800˚C and 1000˚C with a dopant concentration of 1%. Characteristic agglomerated morphology is confirmed in $Ca_3(PO_4)_2$ and $Ca_3(PO_4)_2$:Ce^{3+} at both temperatures. Irrespective of the dopant addition and annealing temperature, the materials are having β-TCP, rhombohedral structure(R-3c,167). Photoluminescence (PL) studies confirmed the broad emission peaks correspond to the 4f-5d transition of Ce^{3+}. The broad emission and excitation peaks are deconvoluted, which corresponds to the characteristic transitions, $^2D_{3/2} \rightarrow {}^2F_J$ (J=5/2,7/2) of Ce^{3+}.

c0083

Role of Sacrificial Agent in Improving Electrode-Electrolyte Interface Kinematics in Electrochemical Devices

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The electrode-electrolyte interface kinematics i.e. the charge transfer and the diffusion process between the electrolyte ions and the electrode material plays an important role in deciding the overall performance of electrochemical devices. Electrolyte significantly helps in improving the diffusion process, transport of charges and mass transport process from electrode to electrolyte and vice-versa. Thus, performance of electrolyte is needed to be improved which can be achieved by adding suitable sacrificial agents to electrolyte solution. In order to study the effect of sacrificial agent on the electrode-electrolyte kinematics, a three-electrode measurement system was used and the following electrochemical techniques were performed including Cyclic Voltammetry (CV), Linear Sweep Voltammetry (LSV) and Electrochemical Impedance Spectroscopy (EIS). On the addition of 0.1 M Na_2S as a sacrificial agent in 0.5M Na_2SO_4 electrolyte solution, the current density in LSV is much enhanced, lowering of onset potentials takes place in CV scans and decrease in series and charge transfer resistance is measured in EIS. This improvement in the behavior of an electrochemical system on addition of sacrificial agent is investigated in the present study. Further, as synthesized Cadmium Sulphide Nanoparticles (CdS NPs) used as working electrode material are found to possess hexagonal morphology from Transmission Electron Microscopy (TEM) images and average particle size measured using imageJ software is found to be 12.04±2.79 nm.

c0084

Detection of Dye Molecules Through Photonic Crystal Assisted Surface Enhanced Raman Scattering

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Thin (monolayer) Photonic crystals fabricated through the self-assembly of monodisperse silica colloidal particles are used for the detection of hazardous dye molecule, Rhodamine 6G (R6G) via Surface-Enhanced Raman Scattering (SERS) technique. The silica colloidal photonic crystal monolayer is decorated with gold nanoparticles, synthesized through laser ablation, to make it SERS active. Our results show that the photonic crystal-gold nanoparticle template provides an excellent SERS enhancement in the trace molecular detection of R6G. Electromagnetic simulations were carried out to understand the effect of photonic crystals on the electric field enhancement with and without gold nanoparticles. It is observed that, when gold nanoparticles are placed at the high electric field region of the silica photonic crystal monolayer, the electric field gets further enhanced, contributing significantly to the enhancement of the SERS signal which in turn, push the detection limit to ultra-low concentrations of dye molecules.

c0085

Investigation of structural and Terahertz-based optical properties of Fe-substituted $CuCr_2O_4$

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Nanoparticles of $CuCr_2O_4$ and Fe substituted $CuCr_2O_4$ are synthesized by sol-gel method and characterized with the help of XRD and terahertz to determine the structural and particle size of nanoparticles and optical (electrical) conductivity properties. The XRD results of the parent compound and Fe-substituted $CuCr_2O_4$ exhibited the tetragonal phase and Fe substituted at Cr site, phase transferred o cubic. The analysis of the Terahertz spectra of the compounds showed a decrease in absorption, refractive and dielectric constants with an increase in the Fe content in the series. Consequently, the electrical conductivity of the compounds was calculated and it was increased with an increase in Fe content in the series.

c0086

Investigations of structural, optical and magnetic properties of cobalt ferrite nano-catalyst for water splitting applications

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A possible method for producing environmentally friendly, massive amounts of hydrogen as a sustainable energy alternative is electrocatalytic water splitting. This work examines the electrocatalytic oxygen evolution reaction (OER) behavior of Cobalt Ferrite ($CoFe_2O_4$) nanoparticles produced using wet chemical techniques. The formation of a single-phase cubic spinel structure was verified thorough X-ray diffraction technique. The structural, morphological, textural, optical, and magnetic characterizations using conventional methods. It was found that crystallites were 25 nm in size on average and the lattice constant, X-ray density and other structural parameter were in reported range. The average grain size determined through SEM analysis was of the order of 75 nm and are spherical in nature. EDX analyses confirmed the successful nucleation of $CoFe_2O_4$ to form monophasic. The absorbance bands located at 542 cm^{-1} and 390 cm^{-1} in FTIR spectrum are indicative of characteristics feature of spinel ferrite. The Band gap determined through Tauc plot reflex the semiconducting nature of prepared sample. The magnetic data recorded using VSM technique shows typical hysteresis curve with saturation magnetization 70.94 emu/gm and corecivity of 1.4 KOe. The obtained data on structural, morphological and magnetic characterizations revealed that the prepared cobalt ferrite nano-catalyst can be useful for water splitting application using electrocatalytic process.

c0089

Thermoluminescence Study of Co-60 Gamma Irradiated Anhydrous Polyhalite Synthesized Using Hydrothermal Method

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Anhydrous Polyhalite $K_2Ca_2Mg(SO_4)_4$ nanoparticles were synthesized using hydrothermal method. The obtained nanomaterial is subjected to powder X-ray diffraction for confirmation of its crystal structure. The sample is irradiated by Co-60 gamma radiation with different doses such as 0.5, 1, 3, 6, 10 kGy. The thermoluminescence (TL) reader is used to characterize the synthesized nanomaterial after gamma irradiation. The sample shows good sensitivity for different gamma radiation doses. The sample irradiated with 10 kGy is characterized up to 325ºC at variable heating rates of 1, 2, 3, 4 and 5 K/s. The thermoluminescence glow curve obtained by heating the sample at heating rate of 1 K/s shows single prominent peak at 446 K. This glow curve is deconvoluted using computerized glow curve deconvolution (CGCD) method with figure of merit 1.99%. The deconvoluted curve contains nine distinct peaks at 378, 381.4, 410.1, 430, 445.1, 449.5, 470.25, 506.5 and 557.5K. The glow curve follows general order kinetics. The obtained trapping parameters like activation energy, frequency factor by TL analysis of glow curve confirm that the synthesized nanomaterial is suitable for dosimetric application.

c0090

Engineering Highly Stable $CsPbBr_3$ Perovskite Nanocrystals with Superior Aqueous Fluorescence for Efficient Hg^{2+} Detection in *In-Vitro* Cellular Imaging: The Impact of Surface Ligands and Silica Encapsulation

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Recently, fluorescent $CsPbX_3$ (X = Cl, Br, I) perovskite nanocrystals (NCs) have been explored for the qualitative and quantitative measurements of heavy metal ions. The excellent multiphoton absorption property of the perovskite NCs also allows the integration of infrared light for fluorescent bioimaging applications. However, the poor structural stability of the perovskite materials against water, intense UV-irradiation, and leaching of Pb-ions into the environment remain great challenges for practical applications. In this regard, we encapsulated the $CsPbBr_3$ NCs with silicone oxides to improve NCs' stability while maintaining superior emission properties. These NCs were executed as a fluorescent probe for the detection of Hg^{2+}-ions in water. Finally, these NCs were tested for sensing Hg^{2+}-ions inside the living cells, which demonstrates superior sensitivity for Hg^{2+}-ion detection.

c0091

Synthesis and Characterizations of γ-Graphyne: Advanced 2D Synthetic Allotrope of Carbon

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Recently, Graphyne family is studied extensively owing to their unique structural and physical properties. These are two dimensional (2D) layered man-made allotropes of carbon having both sp^2 and sp hybridized carbon atoms. Among graphyne family, γ-graphyne has aroused a strong interest among researchers due to their fascinating physical properties such as high flexibility, tuneable electronic structure, direct bandgap, low thermal conductance, excellent carrier mobility (10^4-10^5 cm^2/ V s), high surface area with nanoporosity etc. Herein, we have synthesized γ-graphyne by palladium catalysed chemical route and studied their structural and morphological behavior by employing Raman spectroscopy, X-ray diffraction (XRD), nuclear magnetic resonance (NMR), scanning electron microscopy (SEM) and atomic force microscopy respectively. On the basis of above results, it is conjectured that γ-graphyne could be a significant candidate for research and industrial applications like catalyst, sensors, energy storage and harvesting system, microwave absorption and so on.

c0092

Charge transfer process in $CsPbBr_3$ nanocrystals and nitrogen-doped carbon quantum dots heterostructure: effect of nanocrystals' encapsulation Smaranika Ray[1*,] Saikat Bhaumik[1]
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Recently, lead halide perovskite nanocrystals (NCs) based heterostructures have demonstrated significant promise in various research areas, including solar cells, CO_2 reduction, and photocatalysis. These hybrid structures have also played a crucial role in advancing our fundamental conception of charge transfer mechanisms occurring at the interface. A thin shelling around the NCs is not suitable for the formation of stable and luminescent materials. Thick-shelled NCs are highly stable but hinder charge transfer among the NCs which are useful for bio-imaging and color-converted LED fabrication. So, understanding the mechanism of charge transfer depending on the shelling materials is important. Here, we synthesized $CsPbBr_3$ NCs with various coating materials to vary the effective distance between the perovskite and nitrogen-doped carbon quantum dots (NCQDs) to understand the rate of charge transfer between them. We observed that the charge transfer rate between thick-shelled NCs and NCQDs is slow. The faster charge transfer among the thinner-shelled NCs and NCQDs is feasible due to the bonding of the N-state of NCQDs with Pb-atoms of the $CsPbBr_3$ structure. This study held immense significance as it provides crucial insights into the design and application of heterostructures, which can be extended to various novel opportunities for progress and innovation.

c0093

Effect of Humidity on Ammonia Gas Sensing by Hydrothermally Synthesised Gallium Oxide Nanoparticles

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The Gallium Oxide Hydroxide (GaOOH) powders were synthesized by hydrothermal method using Gallium Nitrite Hydrate ($Ga(NO_3)_3$. xH_2O) as precursor at 120℃. The obtained product was calcinated at 1000℃ to get β- Gallium Oxide (β-Ga_2O_3). The resulting product was studied using various characterization techniques such as X-ray diffraction (XRD), scanning electron microscope (SEM). Following XRD analysis, the powder samples revealed polycrystalline nature with monoclinic crystalline structure. The micrographs of powder samples resulted from SEM investigations showed elongated rod morphology. The synthesized β-Ga_2O_3 powder samples were drop casted on glass substrate which was pre deposited with Inter Digitated Electrode pattern (IDE) of Silver (Ag) using evaporation method. This drop coated thick films are then used for the different concentrations of Ammonia (NH_3) vapor detection at room temperature and at various humidity conditions. It has been observed that the β-Ga_2O_3 film showed highest response of 160% under relative humidity of 69%.

c0094

Structural, Optical, Morphological and Electrical Characterization of Nickel Ferrites Thin Film Deposited by Spray Pyrolysis technique

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The spinel ferrite thin film has been prepared on to ultrasonically cleaned amorphous glass substrate at a constant temperature of 360ºC by using chemical spray pyrolysis technique. The prepared films were characterized by X-ray diffraction, Raman spectroscopy, Scanning Electron Microscopy, UV-Vi's spectroscopy studies. The X-ray diffraction patterns confirmed single phase cubic spinel structure with space group of Fd-3m o7h. XRD study revealed, cubic phase formation of polycrystallineNiFe2O4 thin film with crystallite size of 19 nm. Metal cation active vibration modes, metal oxygen stretching and bending vibrations were confirmed through the Raman analysis. The bandgap energy curve indicates direct allowed

bandgap transition with band gap energy (Eg) found to be 2.06 eV. FESEM shows the uniform, compact, spherical, mesoporous, well-grown grain like surface morphology. I-V characteristic curve shows the ohmic nature of the deposited thin films.

c0095

Enhanced Thermal Conductivity And Photo-thermal Conversion in Carbon Black Nano-inclusion Loaded Organic Phase Change Material For Thermal Energy Storage

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Significantly high enhancements in thermal conductivity and photo-thermal conversion is reported for lauric acid-based form-stable phase change material (PCM) loaded with carbon black nano-inclusions (CBNP). Thermal conductivity enhanced by ~ 195 % for the PCM loaded with ~ 3.5 wt. % CBNP nano-inclusion, which is attributed to the formation of interconnected percolation networks during freezing. Addition of ~ 25 wt. % $CaCO_3$ powder to the PCM is found to arrest the material leakage during solid-liquid phase transition due to the capillary action. Photo-thermal conversion efficiency is found to increase by ~ 134 % for ~ 3.5 wt. % CBNP loading, which is attributed to the augmentation of extinction efficiency due to multiple scattering from the CBNP clusters within the host matrix. The excellent photo-thermal efficiency, high thermal conductivity and superior form-stability makes the CBNP loaded LA-based PCM a potential candidate for thermal energy storage applications.

c0096

Effect of Manganese Doping on the Optical Properties of $CsPbBr_3$ Nanocrystals

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Inorganic perovskites present a potential alternative to hybrid organic-inorganic perovskites in the realm of optoelectronic applications due to their heightened stability and distinctive optical and electronic properties [1]. Introducing dopants stands out as a promising approach for tailoring the optoelectronic characteristics of these perovskite nanocrystals (NCs), owing to the robust exchange interaction between dopant ions and host NC excitons [2-3]. In the present work, successful synthesis of $CsPbBr_3$ NCs with blue emission is reported. Subsequently, we embarked on a strategic doping wherein Mn^{2+} ions were introduced into the $CsPbBr_3$ NCs, specifically occupying Pb^{2+} sites. A comprehensive investigation of the resulting changes in photoluminescence (PL) properties before and after the doping was carried out. Initially, CsPbBr3 NCs was synthesized followed by the doping of Mn^{2+} ions via an immiscible bi-phasic method, facilitated by the presence of the electron-donating oleylamine ligand. A perceptible shift in colour, transitioning from blue to a pinkish hue was observed coinciding with a detectable broad hump in the photoluminescence spectrum spanning from 550 nm to 650 nm [4]. These findings will contribute significantly to the progression of the comprehension of efficient metal ion doping for optoelectronic applications.

c0097

Rare Earth Composited With Green Synthesized Carbon Dot towards High Dielectric Nano Materials

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In this paper, we report a huge increment of the relative permittivity of PMMA-based nanodielectrics in the presence of carbon dots (CD) and Neodymium-doped carbon dots (Nd-CD). 10wt. % of CD and Nd-CD were composited with PMMA to form PMMA@10CD and PMMA@10Nd-CD nanocomposite films, and these films were characterized by different techniques. The dielectric response study specifies the remarkable enhancement of relative permittivity of PMMA in the presence of CDs (~15 times), and this value is increased further in the presence of Nd-CD (~153 times). As the temperature increases, the effective dipolar polarization of the composites increases, which in turn give assistance to enhance the relative permittivity. Nevertheless, at 75°C and 100Hz, the relative permittivity value for PMMA@10Nd-CD composites reaches nearly 1242 (234 times), the highest reported PMMA composites to date. In this study, the unique and sensitive change in dielectric and electrical properties of PMMA-based nanodielectrics was observed, which is helpful in the commercial use of PMMA nanodielectrics inside the capacitor.

c0098

Effect of Bandgap on Photocatalytic activity of GO Based Cr Doped NiO Nanocomposites

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In the current study, co-precipitation method was used to preparation of GO-based Pure NiO and 6% Cr-doped NiO nanocomposites. Field Emission Scanning Electron Microscopy (FESEM) and x-ray diffraction (XRD) techniques were used to investigate the impact of Cr doping on the structural characteristics of nanoparticles. The sample's crystalline and crystal structure were evident in the XRD spectrum. Nanoparticle morphology is observed using FESEM. EDAX spectroscopy was utilized for elemental analysis. Optical characteristics were confirmed by using UV-Vis spectrometer. The distinct features of GO based 6% Cr-doped NiO nanocomposite synthesized by co-precipitation has utilised in dye degradation.

c0099

Sonication Assisted Synthesis of $LaFeO_3/Fe_2O_3$/Activated charcoal Nano composite for Photocatalytic Degradation of Methylene Blue Dye

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The pure nano $LaFeO_3$ and Fe_2O_3 is prepared by solution combustion method using glycine as fuel and activated charcoal by thermo-chemical activation method. A ternary nano composite of all these three components is then prepared by simple sonication method. The prepared nano composite is characterized by XRD, UV-Visible spectroscopy, SEM and EDS. The effectiveness of the prepared nano composite is then studied for photocatalytic degradation of methylene blue dye. The results showed that the prepared composite material degraded 5 ppm methylene blue solution by about 56% in two hours under visible light irradiation.

c0101

Green Synthesis Of Zno:Nio Nanocomposite And Its Potent Antibacterial Properties

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The current work examined the antibacterial characteristics of zinc oxide nanoparticles and ZnO:NiO nanocomposite with 5% and 10% NiO from Phyllanthus Emblica fruit extract. Escherichia coli, Staphylococcus aureus, Pseudomonas aeruginosa, and Bacillus subtilis were tested for antibiotic activity using the agar well diffusion method at 1000 ug/mL nanocomposite. XRD and FESEM were used to characterize the nanocomposite. XRD shows ZnO (hexagonal) and/or NiO (cubic) phases with typical crystallite sizes of 21 and 18 nm, respectively. The morphology is hexagonal on FESEM pictures. Zn-O and Ni-O stretching frequencies are shown by FTIR. The 10% NiO nanocomposites showed strong antibacterial activity against two bacterial strains: Gram-positive Staphylococcus aureus (32 mm) and Gram-negative Pseudomonas aeruginosa (35 mm).

c0102

Ion beam alignment of Au/ZnO nanostructures and UV-Visible Absorption Studies

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In this paper, we examined the surface morphology and the UV visible absorption properties of ion beam modified Au/ZnO composites. ZnO thin film is deposited onto the Si substrate using pulse laser deposition technique and Au NPs are topped onto it via magnetron sputtering. ZnO/Si and Au/ZnO/Si films are irradiated by Xe^+ ions with fluency of 1×10^{16} ions/cm^2 and 70^0 as a glancing angle. The SEM micrographs of the irradiated samples show the highly aligned unidirectional nanopinstripes. The enhancement in the near band edge absorption spectra of ZnO is seen in irradiated Au/ZnO nanoparticles and broadening of localized plasmon band in the visible region.

c0103

Surface Functionalized CuS Nanoparticles for Chemo-photothermal Therapy

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Photothermal therapy (PTT) is a new treatment modality for cancer. In this aspect, water-dispersible phosphate functionalized CuS NPs (PCuS NPs) were developed by soft chemical approach using sodium hexametaphosphate (SHMP) as a stabilizing agent. The successful formation of covellite CuS phase with average size of about 5 nm was confirmed by XRD and TEM analyses. The functionalization of CuS NPs with SHMP was evident from FTIR, dynamic light scattering (DLS) and zeta potential measurements. The UV-visible absorption spectra of PCuS NPs showed broad absorption band in the range of 650-1350 nm with maxima ~920 nm, thus can be used for NIR induced PTT. PCuS NPs showed excellent heating efficacy under excitation at 980nm. Moreover, these negatively charged NPs were conjugated with positively charged anticancer drug, doxorubicin hydrochloride (DOX) through electrostatic interaction. The drug loaded system revealed pH dependent release

behaviour with higher at mild acidic environment. From in-vitro studies, it has been observed that the developed PCuS NPs retained therapeutic efficacy of DOX. Specifically, the present study demonstrated the development of aqueous stable CuS NPs and their heating efficacy.

c0105

Nickel Oxide Nanoparticles as A Photocatalyst for Solar Energy-Mediated MB Degradation

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The primary objective of this study was to explore the influential factors governing the photocatalytic degradation of wastewater using bio-synthesized nanoparticles of Nickel oxide (NiO-NPs) within aqueous solutions. Among the spectrum of semiconductor oxides, nickel oxide stands out for its robust chemical stability and pronounced catalytic prowess, rendering it an exceptional candidate as a photocatalytic material for eco-friendly applications, specifically in wastewater degradation. In the course of our investigation, we meticulously scrutinized a range of variables, notably the irradiation duration, during the degradation process. Our analysis of NiO-NPs revealed a discernible band gap of 2.65 electronvolts through UV-Vis spectroscopic characterization. Microstructural analysis through Scanning Electron Microscopy (SEM) unveiled irregular and agglomerated morphologies, with a predominant spherical shape. This was further corroborated by X-ray Diffraction (XRD) characterizations, which confirmed the presence of a cubic crystal structure. This study thus presents an exhaustive assessment of the photocatalytic degradation of wastewater employing NiO-NPs in conjunction with ultraviolet (UV) light irradiation for effective wastewater treatment. Impressively, the results showcase a striking 95% degradation efficiency in dye content after a mere 140 minutes of exposure, further demonstrating commendable resilience with an 85% degradation efficiency even after the third repeated cycle, attesting to its sustained durability

c0106

Upconversion Nanoparticle embedded SiO_2 Nanospheres for Anticancer Drug Delivery

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Lanthanides (Yb: 20%, Er: 2%) doped calcium fluoride (CaF_2) upconversion nanoparticles (UCNPs) were prepared by miniemulsion method and encapsulated them into mesoporous SiO_2 nanospheres (UCNP@m-SiO_2 NSs) for anticancer drug delivery. XRD and TEM analysis revealed the formation of highly crystalline cubic phase fluorite-type nanostructure. These nanospheres are highly mesoporous in nature, and possess high surface area and good aqueous colloidal stability. Photoluminescence studies showed emission peaks in visible region upon 980 nm excitation, indicating strong upconversion capabilities of the nanospheres. The anticancer drug, doxorubicin hydrochloride (DOX) was successfully loaded into the mesopores of UCNP@m-SiO_2 NSs and the DOX loaded system (DOX-UCNP@m-SiO_2 NSs) exhibited pH dependent drug release profile with higher release at mild acidic environment. The drug loaded system retained therapeutic efficacy of DOX and showed a dose-dependent toxicity towards breast cancer (MCF-7) cell line. Specifically, the present study demonstrated the development of water-dispersible and biocompatible luminescent nanocarriers for anticancer drug delivery.

c0107

Development of highly flexible and cost-effective cello tape-based surface enhanced Raman spectroscopy (SERS) substrate with extremely high sensitivity

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The competitive study aims to develop a highly flexible and cost-effective cello tape- based surface-enhanced Raman spectroscopy (SERS) substrate for rapid detection of ultralow concentration of analytes. Flexible substrates have an advantage over rigid substrates as they exploit the ability to conform with underlying surface and can easily be modified to any shape, size based on their applications. SERS has matured into a versatile technique ideal for detection of chemical and biological molecules. The ability to enormously amplify the Raman signals in close proximity to the plasmonic nanostructures is the selling property of SERS based detection. The AgNR array substrate fabricated on flexible cello tape surface using physical vapor deposition technique GLAD. This oblique angle deposition (OAD) technique is facile method for fabricating high-end Ag nanorods for obtaining best SERS enhancement.
Characterization nanostructures fabricated on flexible cello tape AgNR based substrates was done using FESEM, TEM, EDX, XRD and UV-Vis. The characterization showed successful growth of pristine AgNR columnar structures on the very flexible cello tape surfaces. SERS spectra of Rhodamine 6G (Rh6G) dye on AgNR embedded cello tape substrates was obtained. SERS measurements of Rh6G with different conc. ranging from 10^{-6} M to 10^{-15} M were preformed to test the sensitivity of substrates. Femtomolar level detection was obtained using these novel substrates showing its immense sensitivity. Because of the high flexibility, our SERS substrates can find "paste and peel off" applications in sensing, single molecule detection and other real-world problems.

c0108

Design and Development of Arduino Based Data Acquisition System for ZnO Nanowires based NO Sensors

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We report the design and development of multichannel Arduino based data acquisition system with programmable temperature that can be used for both data acquisition and final sensors device, when ready. The system has the provision of setting the temperature of 4 sensor heads/units to the desired temperature from RT to 250°C. This is achieved using the simple program written in Arduino Programming Language available via Arduino Desktop IDE. Importantly, the developed unit could be used to record the resistance changes from 20 MΩ to 1 kΩ. The system has been tested and validated using ZnO nanowires based NO sensors.

c0109
Barium Manganese Titanate (Ba_2MnTiO_6) Double Perovskite Based Phosphor
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Over the years, Eu^{3+} activated phosphors find important place in the fabrication of white LEDs (WLEDs)as the main red emitting material. Double perovskites doped with Eu^{3+} have attracted researchers for enhancing the overall performance of WLEDs. Considering this, we prepared Ba_2MnTiO_6 by high temperature solid state reaction method in air and its potential for red phosphor is studied by doping with Eu^{3+} ions. The prepared compound was confirmed by XRD study. Vibrational nature was observed from its FTIR spectra. Absorption and emission characteristics will also be discussed.

c0110
Bare SnO_2 QDs based Ammonia Sensing at Room Temperature in Humid condition
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Abstract: Uncapped SnO_2 quantum dots with an average crystallite size of ~2.4 nm were synthesized by a soft chemical route for developing room temperature ammonia sensor. SnO_2 QD slurry was deposited on the interdigited Au electrodes for resistive study. The resistive sensor showed a strong decrease in the resistance on exposure to ammonia hydroxide at room temperature. The SnO_2 QDs sensor worked in a wide range of humidity and showed repeatability and recovery with high sensitivity. Moreover, it could perform at a high concentration of ammonia hydroxide. The sensing mechanism indicated the critical role of surface defects and hydroxyl groups of SnO_2 QDs. The Raman spectrum after exposure of NH_4OH is recorded with a 325 Laser excitation. Distinct fluorescence background was observed for only NH_4OH at ambient conditions. This optical probe in combination with resistive change provides high selectivity for NH_4OH.

c0111
FM-Exchange Coupling Induced Uniaxial Anisotropy in a System of Cobalt Carbide Nanoparticles- A Micromagnetic Simulation Study
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Abstract. We micromagnetically simulate the exchange bias (EB) effect in a simplified bilayer form for a system of cobalt carbide (Co_2C) nanoparticles having a core-shell structure. The sample consists of a ferromagnetic (FM) spin block exchange coupled to a single layer of disordered spins (DS). Coercivity decreases while EB increases with the FM-DS interfacial exchange coupling strength. We roughly estimate the exchange coupling energy at the interface which is difficult to probe experimentally. EB also increases linearly with the net uncompensated moment at the FM-DS interface. The total exchange coupling energy dominates the anisotropy energy concomitant with the EB appearing in the system. Through a numerical model, we establish that the interfacial exchange coupling energy not only contributes to the EB effect but also gives rise to an additional anisotropy that may enhance the superparamagnetic blocking temperature of the NPs.

c0112
Fine Tuning of the Electronic and Structural Defect Properties of Wide Bandgap Semiconductor Nanocrystallites; Pure and Zn-Doped CdO as Case Studies
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Cadmium oxide nanocrystallites, pristine and zinc-substituted, were synthesized using chemical precipitation method. X-ray diffraction revealed the characteristics peaks with the expected 2θ values and finite broadening. In the undoped series, the average nanocrystallite size increased from 16 nm to 30 nm due to agglomeration while, in the Zn-substituted samples, it decreased from 25 nm to 16 nm due to the smaller radii of the substituted Zn^{2+} ions than the host Cd^{2+} ions. Positron lifetime and coincidence Doppler broadening measurements were used to identify Cd^{2+} monovacancies as the dominant type of defects, although thermal diffusion to the nanocrystallite surfaces reduced positron annihilation within the nanocrystallites. The segregation of ZnO at higher doping concentrations paved the way for interfacial defect formation that resulted in increased positron trapping.

c0113

Exploration of the Defects in Pure and Cerium Doped Bismuth Ferrite Nanocrystallites

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Bismuth ferrite (BFO) nanocrystallites, both pure and cerium-doped, are synthesized by sol-gel method. The systematic variation in the duration of calcination at 600 °C resulted in different sizes of nanocrystallites. X-ray diffraction studies showed the formation of *R*3*c* phase of BFO and the varying sizes of the nanocrystallites. Positron annihilation spectroscopy monitored the defects dynamics. Majority of the positrons annihilated from the surfaces in smaller nanocrystallites. In the crystallites of sizes larger sizes, positrons got trapped in Fe^{3+}/ Bi^{3+}-O^{2-} divacancies. The coincidence Doppler broadening spectroscopic experiments also indicated the presence of divacancy clusters. In the Ce^{3+}-doped samples, positron annihilation at the nanocrystallite surfaces dominated over that at the defects within the nanocrystallites.

c0114

Abstract.

Synthesis, Structural and Photocatalytic Studies of $MnCo_2O_4$ – CuO Nanocomposites

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Visible light driven photocatalysts $MnCo_2O_4$ and CuO were successfully synthesized via co- precipitation route. Their respective nanocomposites were prepared in the ratios 9:1, 8:2 and 7:3 via solid state route. The synthesized compounds were characterized by X-Ray diffraction and Diffuse Reflectance Spectroscopy (DRS). These nanocomposites were further subject to photo-catalytic studies under various conditions and the optimal parameters were obtained. The optimized Nanocomposites photocatalyst was further experimented on different dyes to check its versatility. It showed promising photocatalytic activity for numerous dyes. The photocatalytic efficiency was further increased to almost 100% with enhancement of catalyst by addition of trace amounts of H_2O_2. The obtained results clearly show excellent photocatalytic activity of the synthesized nanocomposites.

c0115

The Scherrer Equation: Limitations and Remedy

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The Scherrer equation is an integral part of various diffraction based methods of microstructural analysis. This equation is used for accounting diffraction peak broadening contribution arising due to crystallite size-effect part of nanomaterials. It has two major limitations: (i) it gives apparent mean (related to volume-weighted average) crystallite size only and does not tell about size-distribution of the crystallites (which modifies the diffraction peak shapes). (ii) Usually different values of mean-crystallite sizes are obtained from the same diffraction pattern depending upon the definition of peak width i.e. Full Width at Half Maximum (FWHM) breadth and Integral Breadth (IB). In this work it is shown that knowledge of peak shape information solely due to size-effect can be used to rectify these limitations of the Scherrer equation. Also the differences in the FWHM and IB based Scherrer constants (which are frequently considered as same) are explained using peak shapes.

c0117

Preparation and characterization of Nano composites of Fe Complex using Aniline based Schiff base Ligand (P - chloro-salicylidene Aniline)

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Abstract. The present study focuses on the formation of Nano composites Fe (II) complex using Schiff base ligand which derived from P - chloro-aniline and Salicylaldehyde because Schiff base and their metal complexes hold significant properties as catalysts in various biological systems, antimicrobial activities, antifungal activities, antitumor and antiviral activities. After the formation we used Fourier transform infrared spectroscopy (FTIR) to obtain information about the various functional groups and the possible chemical structure of the Complex because vibrational spectroscopy plays a significant role in providing that information. The synthesized Fe (II) complex was also characterized by X-Ray diffraction (XRD) for get the crystalline state of the complex and scanning Electron microscope (SEM) to get information about the surface morphology of the complex.

c0119

Carbon Nano-corals Synthesized Through Chemical Vapor Deposition

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Abstract

Carbon nano-corals (CNcs) are synthesized on copper strips by thermal Chemical Vapor Deposition (CVD), using Acetylene (C_2H_2) as precursor and Argon as carrier gas. Microstructural analysis of the grown structures is carried out by Field Emission Scanning Electron Microscopy and RAMAN spectroscopy is done to analyze the graphitic carbon content. Star and grooved brain coral like structures are observed which may have formed due to stacking and rolling of graphene sheets. The characteristic D and G peaks in RAMAN spectra corresponds to graphitic carbon. The highly porous structure of the carbon nano-corals has a potential for hydrovoltaic application.

c0120

Surface Functionalized Metal Nanoparticle Conjugates with Nanocavitands: Applications in Drug Delivery

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Abstract: Thioflavin-T (ThT) is a cationic dye that is commonly used to detect the formation of amyloid fibrils in tissues, which is associated with chronic diseases such as Alzheimer's and Parkinson's[1]. ThT specifically binds to protein fibrils, and its fluorescence increases significantly upon binding to the cavities in the amyloid fibrils, making it a highly sensitive and versatile tool for detecting amyloid fibrils in tissues. p-sulfonatocalix[6]arene is a highly biocompatible supramolecular host molecule, which is known to stabilize different metal nanoparticles[2]. Supramolecular host capped nanoparticle can have potential application for efficient drug delivery[3].

In this work, p-sulfonatocalix[6]arene (SCx6) capped gold nanoparticles (SCx6AuNP) have been synthesized and characterized. Interaction of this surface decorated cavitands with a model probe thioflavin T (ThT) have been studied by various spectroscopic techniques to evaluate the contribution of nanoconjugate surface towards binding and release of ThT. The fluorescence intensity and lifetime of ThT increase upon gradual addition of SCx6AuNP and attains saturation at very low concentration of the nanoparticles, indicating strong interaction between them. Whereas, AuNPs without SCx6 did not show any interaction with ThT. The stability of the calixarene-coated AuNPs increases as compared to the uncoated AuNPs. Stimuli-responsive behavior of ThT:SCx6AuNP assembly has been examined by using external stimuli such as amantadine hydrochloride and temperature. It is observed that the absorption and fluorescence behavior of the assembly reverts back to those of the free dye. This result suggests the release of ThT dye from the cavity of SCx6 attached to the AuNP and can find potential applications in drug delivery.

c0121

Fe Nanoparticles as Catalytic Scissors to Unzip Carbon Nanotubes

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Abstract. Single wall carbon nanotubes (SWCNTs) synthesized by high pressure carbon monoxide (HiPCO) method contain metal impurities and amorphous carbon which require purification for further use. During the synthesis process of HiPCO SWCNTs, iron pentacarbonyl ($Fe(CO)_5$) is employed as catalyst that plays a crucial role by forming Fe clusters to provide growth sites for the carbon nanotubes (CNTs). Hence, the structure and the morphology of CNTs can be controlled by varying $Fe(CO)_5$ content in the precursors. The route of the purification process and the purity level of the tubes can be decided according to the target application. Here, we report our investigations on the core-shell structure of the Fe catalyst particles in the purified sample with cores formed by different structural phases of iron (Fe) and oxygen (O), whereas the shells are comprised of multiple graphitic layers. These metal particles act as a catalytic scissor to unzip the carbon nanotubes (CNTs), assisting emergence of different low dimensional structural forms carbon [1]. We present here X-ray diffraction (XRD) and high resolution transmission electron microscopy (HRTEM) studies to demonstrate the catalytic action of the core-shell Fe nanoparticles as scissors.

c0123

Effect of Co doped ZnO Nanorods on Photocatalytic Activity

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Pure and Co-doped ZnO nanorods was successfully synthesized by a simple Co-Precipitation method. The structural and surface morphological properties of pure and 1% Co doped ZnO nanorods were investigated by using XRD and FE-SEM respectively. The XRD analysis revealed that as prepared samples exhibit Hexagonal Wurtzite crystal structure. From FE-SEM images it is reflects that the single crystalline nanorods were formed after doping of Co in ZnO lattice. The photocatalytic

activity was performed for the degradation of methylene blue dye which results in the photocatalytic efficiency was increased upto 73% after Co doping.

c0124

SPR-Assisted Enhancement in Visible-Light Driven Photocatalysis of β-In_2S_3 Quantum Dots in Nafion

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In this work, we report the synthesis of β-In2S3, Ag NPs and Ag- In2S3 complex superstructures in a perfluorinated cation exchange membrane (Nafion 117) to produce stable and reusable thin films. The surface plasmons in the metal nanoparticles create enhanced electromagnetic fields which influences the optical characteristics of the surrounding semiconductor quantum dots. Here, we observe an enhancement in the absorption of visible light due to strong plasmon-exciton coupling thus increasing the quantum efficiency of the material. The band gap energy of the composite film shows a blue-shift of 0.65 eV when compared to β-In2S3 film. The XRD reveals a modification in crystal structure of β-In2S3 quantum dots from tetragonal bcc lattice to cubic fcc lattice on incorporating Ag NPs. The films are potential photocatalysts for complete disinfection of sea water and the composite, Ag- In2S3 Nafion film shows the highest rate of disinfection compared to the others as a result of the enhanced optical properties adhering to the exciton-plasmon coupling.

c0125

Performance Enhancement of Co_3O_4@rGO Nanocomposite-Coated Optical Fiber for Acetone sensor

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ABSTRACT: Transition metal composite semiconductor nanomaterials are increasingly popular in gas sensing due to their crystal structure, tunable properties, stability, and surface reactivity. They offer high sensitivity, low detection limits, and applications in environmental monitoring, healthcare, and industrial processes. This research proposes a fiber optic sensor for detecting acetone gas that is based on semiconductor composite nanomaterial coatings. The composite materials, size, and shape are the various factors that can influence sensing properties. XRD and UV-vis spectroscopy techniques used to characterize the structural and optical properties of the prepared Co_3O_4@rGO nanocomposite and used as a coating material on a small portion of unclad glass fiber to design a nanocomposite coated optical fiber sensor (NCOFS). The addition of rGO to Co_3O_4 improves the Limit of Detection (LOD) by 1.5ppm. Further, the sensitivity of detection, response time of the sensor are found as 0.002µA/ppb and 60second respectively. The specificity of the sensor is also investigated for the interfering species like ethanol, methanol and isopropanol.

c**0126**

Investigations on Structural and Electrical Properties of Manganite – Silica Nanocomposites

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In this study, investigations on structural and electrical properties of sol – gel prepared manganite – based nanoparticles of $Dy_{0.7}Ca_{0.3}MnO_3$ and nanostructured SiO_2 based nanocomposites has been carried out. Structural properties have been performed by X – ray diffraction measurement which reveals single phasic nature without any detectable impurity phase in the lattice and crystalline size has been obtained by Scherrer's formula. Electrical characterizations (ε′, □, Z) have been performed using high precision LCR meter in the frequency range of 1 kHz to 2MHz. Variation in dielectric constant has been understood on the basis of Maxwell – Wagner (M – W) mechanism and Koop's theory. Furthermore, dielectric nature has been studied from universal dielectric response (UDR) model and dissipation energy of dipoles from dielectric loss. Frequency dependent variation in ac conductivity explained from Jonscher's universal power law on the basis of correlated barrier hopping (CBH) mechanism. Resistive nature of the lattice obtained from frequency dependent impedance.

c**01**27

Blue-Green Emission in $MoO_3:Tb^{3+}$ nanophosphors: Investigation on the Structural and Photoluminescence Properties

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Abstract. $MoO_3:Tb^{3+}$ nanophosphors were synthesized through hydrothermal method by varying the terbium doping concentrations. The study includes the investigation of structural, optical, and photoluminescence characteristics of $MoO_3:Tb^{3+}$ nanophosphors. Raman spectroscopy and X-ray diffraction analysis were conducted to analyze the crystal structure, vibrational modes, and symmetry of the prepared nanoparticles. The results from XRD and Raman spectroscopy affirmed the orthorhombic phase of MoO_3. From FESEM, nanosheet-like morphology was observed and wide bandgap is obtained from the Tauc plot. Upon exciting $MoO_3:Tb^{3+}$ nanophosphors at 260 nm, a blue-green emission spectrum emerged and quenching mechanisms were observed. The quantification of the blue-green emission was accomplished using the CIE chromaticity diagram. Nevertheless, there is no existing studies that elucidate the photoluminescence characteristics of $MoO_3:Tb^{3+}$ nanophosphors, which is worth investigating. This work provides a detailed analysis of the photoluminescence properties, concentration quenching mechanism and evolution of blue-green emission in $MoO_3:Tb^{3+}$ nanophosphors.

c0129

Studies on Structural and Electro-Transport Properties of Doped Metal Oxide Nanoparticles

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Abstract. In this present research work, we have successfully synthesized Al Doped ZnO nanoparticle samples using wet-chemical method via low-cost sol-gel process at different sintering temperatures of (a) 900 °C (b) 1000°C and (c) 1100 °C referred as (a) ZAO9 (b) ZAO10 and (c) ZAO11. The structural properties have been emphasized by powder x-ray diffraction method which reveals the successful doping of Al at Zn site of structure overall shows the single phasic nature wherein, increment in the sintering temperature leads to sharper XRD peak indicates the improvement in crystalline size in the sample. The microstructural properties of all the samples have been characterized using scanning electron microscopy (SEM) which shows larger morphology at low sintered temperature nanoparticles. Al doped ZnO find great potential application transport conducting oxides hence; its electrical properties i.e., dielectric constant, a.c. conductivity and impedance in the frequency range of 20 Hz to 2 MHz at different temperature range have been studied in vicinity of crystalline size.

c0130

Au Nanoparticles Decorated Titanium Dioxide Nanotube Arrays for Sunlight Driven Photocatalytic Degradation of Trinitrophenol

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In this study, titanium dioxide nanotube arrays (TiO_2) were prepared by two-step anodization. The length and diameter of the nanotube arrays were controlled by varying the duration of anodization. The TiO_2 nanotubes were annealed and subsequently spin-coated by Au nanoparticles (AuNPs). The AuNPs enhanced the visible light activity of TiO_2 nanotubes by localized surface plasmon resonance. The AuNPs-coated TiO_2 nanotubes were characterized using FESEM, XRD, UV-Visible spectrophotometer and photoluminescence spectrophotometer. The photocatalytic activity of AuNPs-coated TiO_2 nanotubes was studied using trinitrophenol degradation under sunlight. The photocatalytic activity depends on the geometry of the AuNPs-coated nanotubes. The nanotubes prepared for 600 s duration showed enhanced photocatalytic degradation of trinitrophenol dye after 180 minutes of duration under sunlight. The enhanced photocatalytic activity of AuNPs-coated TiO_2 nanotubes can be attributed to the combined effects of large surface area of TiO_2 nanotubes and effective visible light absorption by AuNPs.

c0131

Pore Architecture Investigation of Unsubstituted Imidazole Incorporated Hybrid ZIF-8 Synthesized using Delayed Linker Addition Method

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Abstract. Zeolitic Imidazolate Framework-8 (ZIF-8) has gained extensive attention due to its remarkable thermo-chemical stability, and exceptional gas separation capabilities. Introducing unsubstituted imidazole (Im) into ZIF-8, while maintaining its topology and morphology, presents a challenging yet promising strategy for enlarging pore sizes. This enlargement attempt aims to enhance the gas separation performance for larger gas molecules such as n-butane and iso-butane, compared to the pristine ZIF-8. In the present study room temperature delayed linker addition method has been used for the synthesis of Imidazole incorporated ZIF-8. This strategy has led to the incorporation of up to ~ 25 mol% imidazole into the ZIF-8 sodalite structure. The phase purity, crystallinity, topology, morphology, chemical structure, and pore architecture were determined using X-ray Diffraction, Field Emission-Scanning Electron Microscopy, Fourier Transform Infrared, and Positron Annihilation Lifetime Spectroscopy (PALS). The imidazole incorporated ZIF-8 exhibits expanded pore dimensions than pristine ZIF-8, as confirmed by PALS.

c0132

Role of Synthesis Procedure and Solid State Properties of Heat Treated Cobalt Ferrite Nanoparticles

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Abstract. Cobalt ferrite nanoparticles have been successfully prepared by sol-gel method assisted with cow-urine. The stoichiometric of present ferrite system was confirmed from the EDX spectrum. XRD patters revealed the spinel phase of

present ferrite system and amorphous look is more evident in the ferrite systems sintered at low temperatures. Lattice parameter (8.254 – 8.376 Å) and crystallite size (3.7 – 9.7 nm) seems to be increasing with the heat treatment. The grain boundary energy released during the sintering process promoted the crystalline growth. The agglomeration of nanoparticles into large clusters due to strong magnetic interactions is visualized from the nature of SEM.. The results are discussed in terms of thermodynamical considerations.

c135

Structural and Photo Degradation Studies on Ti doped ZnO and TiO_2 – ZnO nano composite Synthesized by Sol-Gel Method

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Abstract. The ZnO and Ti:ZnO nano composites were prepared by sol-gel method using propanal as solvent. The atomic percents (at.%) of Titanium (Ti) doped to ZnO were varied from 2 – 13. The obtained composite is having the Ti composition 7.6 and 12.8. The microstructure confirms the formation of nano composite. The prepared ZnO and Ti:ZnO were crystallizes in Hexagonal wurtzite structure with three predominant (002), (101) and (100) orientations. The photo catalytic response was measured using degradation of methylene blue dye under low power UV lamp irradiation. Pure ZnO exhibits the rate constant of 4.6x10-2 m^{-1} which increased by 20% with formation of TiO_2 – ZnO nano composite with Ti at.% of 12.8. For other Ti dopant concentrations the degradation rate constant decreased attributing to lower crystallite size with higher grain boundaries leading to charge carrier recombination and suppressing the formation of reactive oxygen species. This study reveals importance of crystallite size in dye degradation process. The grown Ti:ZnO and TiO_2 – ZnO nano composite using a simple and scalable synthesis route with hexagonal structure are highly efficient photocatalyst materials for application of waste water treatment in industrial effluents.

c137

Effect of Trivalent Cr^{3+} substitution on Structural, Morphological and Magnetic Properties of Cobalt-Lithium Ferrite Nanoparticles

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Abstract. The present work focuses on structural, morphological and magnetic properties of trivalent Cr^{3+} substituted cobalt-lithium ferrite nanoparticles prepared by cost-effective sol-gel auto combustion method for biomedical applications. The structural analysis of the prepared nanoparticles performed by X-ray diffraction (XRD) confirmed the phase pure nature with nanocrystalline spinel cubic structure formation. The morphological studies performed by scanning electron microscopy depicted the spherical grain formation in the nanometer range. The BET surface area determined from N_2 isotherm curves are found superior as compared to the literature reports. The room temperature M-H hysteresis plots of prepared nanoparticles showed typical ferrimagnetic behavior. M-H curve show superparamagnetic behavior with decreasing saturation magnetization with increasing Cr doping.

c138

Optoelectronic Characteristics of Microwave-Synthesized Cobalt-Doped CZTS for Solar Cell Absorber Layers

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This study presents the successful microwave-assisted synthesis of 5% cobalt-doped CZTS powder. The optical, structural, and electrical characteristics of the synthesized materials were comprehensively evaluated. X-ray diffraction and Raman scattering spectroscopy analyses confirmed the monophase kesterite structure of Co-CZTS with well-defined crystallinity. UV-visible absorption spectroscopy demonstrated an absorption coefficient exceeding 10^4 cm^{-1}. Notably, the optical band gap energy of conventional CZTS decreased from 1.5 eV to 1.4 eV upon cobalt doping. Hall coefficient measurements indicated positive values, signifying p-type conductivity, aligning with the requirements for solar cell applications. This investigation focuses on utilizing Co-CZTS as an absorber layer to mitigate band offset in existing low-efficiency solar cells.

C139

Enhancing the Oxygen Evolution Reaction (OER) Performance by Means of Multi-dimensional Carbon Compounds

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The quest for cost-effective and advanced electrocatalysts to replace precious metal-based ones in the oxygen evolution reaction (OER) holds immense promise for water electrolysis applications. In this study, we present a systematic wet-chemical approach to synthesize a unique hybrid structure combining perovskite oxide ($LaCoO_3$) and various carbon nanostructures including acetylene black (0D), carbon nanotubes (1D), and reduced graphene oxide (2D). This hybrid architecture exhibits significantly enhanced OER electrocatalytic activity compared to the individual components. Detailed material analyses confirm the structural integrity and hybrid nature of the electrocatalysts. The OER performance showcases a lowered onset potential from 1.7 V to 1.6 V and a reduced Tafel slope from 140 mV/dec to 88 mV/dec, highlighting the improved efficiency. Importantly, the $LaCoO_3$/reduced graphene oxide (rGO) hybrid outperforms the 0D and 1D carbon counterparts. This innovative design paradigm could be extended to create hetero-composites comprising diverse perovskite-type oxides and transition metal dichalcogenides (TMDs), thereby laying the groundwork for the development of versatile bifunctional electrocatalysts tailored for water splitting applications.

c140
Theoretical Analysis on Graphene – Ag-MgF_2 Nanocomposite based One-dimensional Photonic Crystal
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The transmission spectra of the proposed one-dimensional photonic crystal (1D-PC) composed of graphene monolayer (layer A) and silver doped MgF_2 nanocomposite (layer B) using the Transfer Matrix Method (TMM) is analyzed. This study demonstrates the tunability of the photonic band gap (PBG) in the 1D-PC structure by controlling various parameters such as the number of periods, fill fraction of the nanocomposite and nanoparticle radius. This has implications for designing photonic devices with specific optical properties, and the observation of an omnidirectional PBG in the ultraviolet to visible range is particularly promising for solar cell applications.

c141
SnO_2 nanostructure based chemo resistive sensor for detection of trace level acetone
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Abstract: In this work, a chemo resistive gas sensor was developed to detect low-concentration acetone vapors using SnO_2 nanostructure. A low-temperature hydrothermal method was employed to synthesize the sensing material. The X-ray diffraction (XRD), field emission scanning electron microscope (FESEM), and transmission electron microscope (TEM) techniques were used to characterize the synthesized material. By carefully drop-casting the sensing material over gold-interdigitated electrodes, the sensor device was fabricated. The sensing performance was investigated in a custom-made gas test system. The sensor is more sensitive towards acetone and able to detect low concentrations of acetone vapors. The response of 23 was obtained in the presence of 20 ppm acetone. The theoretical limit of detection of the sensor is 720 ppb. The proposed sensor is appropriate for monitoring acetone vapors in the indoor environment.

c142
Nonlinear optical studies of Bismuth doped Titanium dioxide nanoparticles
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In recent times, different metal-doped titanium oxide (TiO2) nanoparticles (NPs) are grabbing the attention of the scientific community due to their extended applications in many fields, in particular, optical properties. Bismuth-doped TiO2 NPs were synthesized in the sol-gel method and by dispersing them in ethanol, colloidal dispersions of Bi-doped TiO2NPs were prepared. The nonlinear optical behavior of Bi-doped TiO2NPs was investigated using ultrafast laser pulses of duration ~ 150 fs, repetition rate-76 MHz, at the input wavelengths 700 nm, 750 nm, 800 nm, 850 nm, 900 nm, using the single Z-scan technique. The normalized transmittance traces recorded in both closed-aperture ad open-aperture Z-scan methods were fitted with the theoretical formulae to retrieve the optical nonlinear coefficients (two-photon absorption coefficient, three-photon absorption coefficient, third-order nonlinear susceptibility, intensity-dependent refractive index) Obtained results have demonstrated significantly enhanced nonlinear coefficients compared to pure TiO2NPs in the literature.

c143
Synthesis of In-situ ZnO within PVDF-ZnCl2 Composite: Simultaneous Improvement of Optical And Piezoelectric Properties
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This paper presents an innovative approach for enhancing optical property as well as piezoelectric properties of Poly(vinylidene fluoride) (PVDF) by in situ formation of ZnO within a $ZnCl_2$/PVDF composite. Notably this work reveals the composite's dual increase of optical and piezoelectric capabilities. Synergistic interaction with the PVDF matrix, the ZnO nanoparticles produced within the PVDF matrix leading to enhance optical features and significantly enhance piezoelectric performance by improving β-phase.

c144
Studies on Magnetic Memory Effect and Exchange Bias of Nanostructured Materials
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This article reports studies of exchange bias (EB) and magnetic memory effect of nanostructured materials. Magnetic memory effects in spin-glasses (SG), superspin-glasses (SSG) and superparamagnetic (SPM) materials have been discussed in detail with protocols and mechanisms. The origin of time (t) and temperature (T) dependent magnetic memory effects in different classes of materials have been discussed starting from the nanoscale towards the bulk magnetism. Magnetic memory effects (T and t dependent) in field cooled (FC) and zero field cooled (ZFC) protocols are focused to understand the physics of ageing and rejuvenation in SG, SSG and SPM materials. Exchange bias mechanism in different metal-metal oxide core-shell structures and magnetically inhomogeneous materials are investigated. The dependence of EB with core-shell diameter ration and interparticle interaction are reported which provides a platform to tune EB for potential technological applications.

c145
Synchrotron SAXS study of morphologically modified α-Fe_2O_3 nano-particles synthesized by co-precipitation
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Abstract: Morphological characteristics of technologically relevant nanomaterials are crucial in understanding their unique properties and potential applications. In this study, we employed synchrotron-based Small Angle X-ray Scattering (SAXS) to investigate the structural features of spindle-shaped α-Fe_2O_3 nanoparticles synthesized using co-precipitation method. The synchrotron-based SAXS technique offers several advantages, including high photon flux and enhanced signal-to-noise ratio, enabling us to probe the detailed morphology of the nanostructures. SAXS demonstrates distinct scattering patterns that provide insights into the structural parameters, such as the particle size, shape, and distribution, and correlations among the nanoparticles. The SAXS analysis revealed the presence of well-defined anisotropic features in the nanoparticles, which arises from specific growth processes and self-assembly. The results are further supported by complementary techniques, such as Scanning Electron Microscopy (SEM), confirming the reliability of the SAXS-derived structural parameters. Further, the study demonstrates the capability of synchrotron-based SAXS as a powerful tool for characterizing complex nanostructures, offering a deeper understanding of the fundamental properties that drive the behavior of morphology-property relationships of spindle-shaped α-Fe_2O_3 nanoparticles.

d) Experimental techniques and devices

d0001

Design and Fabrication of Bulk Acoustic Wave Resonator for Magnetic Sensing Applications

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Abstract. The proposed study represents the development of a thin film bulk acoustic resonator, with the ability to detect low magnetic fields with high sensitivity at room temperature. Iron cobalt, a magnetostrictive material with a high magnetostriction coefficient is used as the magnetic sensing layer. The delta E effect is the underline mechanism of magnetic field sensing. Finite element model is used to design the sensor and then resonator is fabricated accordingly. the resultant sensitivity of the FBAR resonator as magnetic sensor is 8.89 kHz/Guass with 18 Guass magnetic field applications. The fabricated sensor has potential applications in biomedical low magnetic field applications.

d0002

Design and Fabrication of Angle Insensitive Transparent Heat Mirror for Energy-Efficient Windows Application

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An easy to fabricate, low cost and effective transparent heat mirror based on dielectric-metal-dielectric thin film stack has been designed and fabricated for radiative cooling application of building windows. Four plasmonic metals visualizing Ag, Al, Au and Cu in combination with high index dielectric layer TiO_2 have been explored through simulation for optimizing the design. Finally, the best optimized design comprising of TiO_2/Ag/TiO_2 layer stack has been fabricated employing ebeam evaporation technique. The transmittance spectra of the developed device are found to be around ~69.1% in visible wavelength range and ~23.2% in the near IR wavelength range. The angle insensitivity of the device has been investigated in the angular range of 0-80$^{o.}$

d0003

Thermal behavior and kinetics of Rice husk blended with Polyethylene terephthalate for co-pyrolysis characteristics

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In this study, we focused on the thermal decomposition, physicochemical properties, thermodynamic parameters and kinetic analysis of the co-pyrolysis process of "polyethylene terephthalate bottles (PET) and rice husk (RH)" which are in the ratio of 1:1 (wt/wt) using thermo-gravimetric analysis at four heating rates of 10 to 40 ^{o}C/min. It has been observed that the co-pyrolysis characteristics of the blends are quite different from the individual materials. Therefore, the potential synergistic effect suggests some chemical interactions between the polyethylene terephthalate and rice husk during the co-pyrolysis process. In this work, kinetic parameters have been analyzed by applying two different iso-conversional methods like Kissinger Akahira Sunose (KAS) and Ozawa Flynn wall (OFW). On the basis of kinetic analysis, it is concluded that both OFW and KAS are equally effective for finding the activation energy and provided the theoretical estimation of the reaction rate and thermal stability of the organic wastes. The present work supports the SDGs of the UN such as Affordable and clean energy (SDG:7), Climate Action (SDG:13) and Life on Land (15).

d0004

Comaparative Study of Response of Synthesized Gd^{3+} Doped $LiAlO_2$ Phosphors With Standard $^{6}LiF/^{7}LiF$:Mg,Cu,P Exposed to Gamma and Thermal Neutron Field.

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In the present work, the Thermoluminescence (TL) response of LAO:Gd ($LiAlO_2$:Gd^{3+}) was investigated after exposure to a n-γ mixed field in the thermal neutron irradiation facility (Standard Thermal Assembly in Graphite). As the neutron field is always accompanied by a photon fraction, some discrimination methodology becomes a primary requirement for quantitative dosimetry and a dosimeter pair with selective response towards both types of radiation is necessary. The discrimination of the two components in the mixed radiation environment was analyzed using a commercially available photon sensitive MCP-(^{7}Li) (^{7}LiF:Mg,Cu,P) dosimeter paired with the LAO:Gd dosimeter to estimate the contribution of individual radiation types in a mixed radiation environment.

d0005

In-situ Cancellation of Ambient Magnetic Field Using Coherent Population Trapping in Atomic Ensemble

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Abstract: The active cancellation of the ambient magnetic field at the atomic vapor cell is carried out by a solenoidal coil and two pair of Helmholtz coil. The coherent population trapping (CPT) signal arising due to interaction of a bi-chromatic light field with atomic ensemble is used for measurement of reference magnetic field. The experiment is carried-out with ^{85}Rb atoms coupled to the light field with D2 transition at 780 nm. The estimation of the bias current through the coils are obtained by iteratively optimizing the strength of the CPT signal for degenerate level. Through a complementary method, the bias magnetic fields (for cancelling ambient field) are calculated from the splitting of the CPT signal by lifting the magnetic degeneracy. The split CPT signal shows distinct spectral profile for longitudinal and orthogonal magnetic field. The separation of split components is a measure of the magnetic field through atomic constants. The measurement by both methods are compared.

d0006

Indigenous Design and Development of Paramagnetic Salt-pill for mK- Resistivity Experiments in QD-PPMS

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De Hass and Wiersma demonstrated the suitability of Chrome Potassium Alum (CPA) for the magnetic cooling method for the first time. The major challenges involved in using the paramagnetic salts for magnetic cooling are their poor thermal conductivity, poor chemical stability at slightly above ambient conditions and corrosivity to metals. This makes the cold finger design very crucial, in deciding the ultimate low temperature that can be achieved. We have developed CPA based salt pills to use it in the commercial Quantum Design-Physical Property Measurement System (PPMS). We have grown the single crystalline CPA in stainless steel cylinder employing the low temperature solution growth technique. For better thermal contact with the cold finger, we have used OFHC copper, about 20 micrometer diameter gold wire strands (in SS salt pill). The OFHC cap is sealed with cylinder using Stycast. To reduce thermal loss further, the pill is mounted on the PPMS puck with polypropylene straw. We could attain the temperature as low as 430 mK in our PPMS. With adiabatic demagnetization technique, we could keep the cold finger temperature between 430 mK- 2K for about 3 hours, which makes its possible application for bolometers also.

d0009

Small-Angle Neutron Scattering Investigations of Laser Host Nd: Y_2O_3 Ceramics

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The pore morphology of transparent and opaque Nd: Y_2O_3 ceramics prepared by co-precipitation (NY-COP) and solid-state (NY-SS) reaction method respectively, has been investigated using small-angle neutron scattering (SANS) technique. The results showed that NY-COP ceramics contain bi-modal pores but NY-SS ceramics have uni-modal pores. Average diameter of pores and concentration in NY-COP ceramics is ~ 123 nm and 5.7×10^{11} cm^{-3} for bigger pores and 31 nm and 8.6×10^{13} for smaller pores. Whereas for uni-modal pores in NY-SS ceramics, these values are ~ 230 nm and 1.5×10^{12} respectively. The total porosity NY-COP ceramics is 0.21 % which is significantly less than that of NY-SS ceramics (0.64%). The optical attenuation coefficients at four wavelengths (λ=300 nm, 450 nm, 645 nm and 1000 nm) are calculated using parameters obtained from SANS and are found to be 34.8 cm^{-1}, 3.5 cm^{-1}, 1.20 cm^{-1}, 0.78 cm^{-1} for NY-COP ceramics. The values corroborate well with experimental values obtained by transmission studies.

d0010

Design of a Continuous Wave Ultrasound Technique to Measure Both the Phase Velocity and Attenuation in Solids

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We developed a simple and versatile non-destructive testing method to simultaneously measure the phase velocity and attenuation of ultrasound wave propagation through solid medium. In this technique, a continuous ultrasound excitation emitting from the high-quality lithium niobate transducer passes through the solid medium and the transmitted signal is received by another identical LiNbO3 crystal. To check the reliability of this method, the velocity and attenuation of both longitudinal and shear ultrasound waves have been measured at room temperature in aluminium and copper correspondingly which are consistent with previous literatures. Moreover, the versatility of this technique has been shown from the phase velocity measurement of the longitudinal excitation as a function of temperature which depicts interesting anomalies across the Verwey transition in Fe3O4 and critical temperature of ferromagnetic ordering in SrRuO3 respectively.

d0011

Investigation of Structural, Optical, Photoluminescence and Colorimetric Behaviors of $Ca_{0.97}Tb_{0.02}WO_4$ Phosphor

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$Ca_{0.97}Tb_{0.02}WO_4$ phosphor has been synthesized by solid state reaction route. Phase purity of the material is confirmed by the X-Ray Diffraction analysis and also denoted that it has tetragonal crystal structure with $I4_1/a$ space group. Lattice parameters of the ceramic are also calculated. Energy band gap value is found from the UV-Visible absorbance spectroscopy. Photoluminescence behaviors of the sample are studied by considering the excitation and emission spectra. Energy transfer diagram is denoted the various electronic transitions that occurred in the material. Emission color with Color Purity, Correlated Color Temperature, Color Rendering Index and Luminous Efficiency of Radiation are calculated by using the CIE Chromaticity coordinates. Quantum Yield Efficiency of the phosphor is observed. Photoluminescence Decay properties are analysed and the average lifetime value is also evaluated.

d0012

Design and Development of IoT based Monitoring System for Smart Agriculture

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IOT based smart agriculture is an emerging technology that leverages the power of the Internet of things to revolutionize the agricultural industry. This technology combines sensor networks, data analytics and automation to optimize crop production, reduce resource wastage, and enhance decision-making processes on the farm. In this paper, we presented a comprehensive view of the various IOT's enabled application in smart agriculture. We explore the key components involved in an IOT based smart agriculture system including sensors, actuators, communication networks and cloud platform. We discuss how these components work together to collect and analyze real -time data on various parameters such as soil moisture, temperature, humidity, light intensity and crop health. Furthermore, we examined the benefits of implementing IOT in agriculture such as crop yield, reduced water and fertilizer usage and enhanced pest and disease management.
We also highlighted the challenges and potential issues faced in implementing IOT based smart agriculture, including data security and privacy concerns, connectivity issues in remote areas and the need for training and education to ensure effective adoption of these technologies. Finally, we presented a case study showcasing the successful deployment of an IOT-based smart agriculture region. We discussed the outcome and input of this implementation, emphasizing the increased efficiency, sustainability and profitability achieved by the farmers.

d0014

The standard molar enthalpy of formation of Bi_2UO_6 and $CdUO_4$ by Micro Reaction Calorimetry

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The standard molar enthalpies of formation of $CdUO_4$ and Bi_2UO_6 were determined by measuring enthalpies of dissolution of by using micro reaction calorimeter at 298 K .The accuracy and precision of these measurements were established with the help of appropriate calibration experiments using pure KCl. The uncertainty in the present measurement is estimated to be within ±.3%. The standard enthalpies of formation of $CdUO_4$ and Bi_2UO_6 at 298 K are found to be **-1457.1** and **-1860.8**kJ mol^{-1}respectively. These data are being reported for the first time.

d0017

VOC sensing characteristics and mechanism of Perovskite Ferrite: Experimental and Theoretical Insights

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Formalin (HCHO), colourless, pungent-smelling gas, widely used in most of industries including chemical, furniture, textile, construction, printing and cleaning industry. Exposer to excess HCHO atmosphere cloud exceled different health problems. Here in, lanthanum ferrite (LFO) based formalin sensor is reported in this work. Lanthanum ferrite was synthesized in hydrothermal method which was used to fabricate Taguchi type chemiresistive sensor. As synthesized material was characterized using several sophisticated techniques (viz. XRD, SEM, EDX, UV-Vis, BET). The experimental results indicated that the fabricated sensor shown good linearity in low ppb range of formalin (CH_2O) gas. The sensor exhibited very high P-type response (~3.25 folds) towards 1 ppm in 30 s at optimal operating temperature of 300 °C. Sensor also showed good selective response towards formalin among other interfering gases for at least 100 days with negligible variation in response. Enhanced sensing response attributes to the favourable charge transfer at LFO interface under exposure of formalin gas which leads to modulate the energy band structure. This study shows that the simple, cost-effective synthesis method along with easy-fabricated and deployable sensor can be applied in many industrial and environmental applications.

d0018

Structural and Luminescent Properties of Dysprosium Doped Niobate Phosphor for W-LED Applications

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A new phosphor based on niobate, doped with Dysprosium, was synthesized via a high-temperature solid-state reaction at 1300°C for 10 hours. X-ray diffraction (XRD) analysis confirmed that the prepared phosphors were of high purity, exhibiting a tetragonal system with the space group P4bm. The surface morphology was examined using field emission scanning electron microscopy (FESEM). To assess the luminescence characteristics, steady-state photoluminescence (PL) measurements were conducted, revealing three distinct emission bands centered at 481 nm, 575 nm, and 666 nm. The influence of Dy3+ concentration on luminescence intensity was also investigated. Moreover, the potential application of the phosphor in w-LED was demonstrated through the study of CIE chromaticity diagrams.

d0019

Behavior Of Microstructural And Electrical Properties Of WO_3 Pellet Processed By Dry Quenching Technique

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Tungsten oxide is considered one of the most beneficial and promising materials in the application fields of photo-electrochemical, energy storage, gas sensors etc. due to its photo-absorption in a broad wavelength range of the near-infrared (NIR) region and efficient light-to-heat conversion, among other properties. In this work, WO3 sample was synthesised by using the cost-effective solid-state reaction technique. After this the pellets were prepared followed by annealing at 800oC for 4 hours. One sample was cooled normally temperature gradient method and other one was by dry quenching method. The structural and morphological studies of both prepared samples were analysed by using XRD and SEM. The formation of a single phase of both WO3 samples were confirmed by using XRD having the peak positions, interplanar spacing, lattice parameters, and volume of the unit cell, with good agreement on the JCPDS file number (01-071-2141) along with the absence of impurity phases. The variations of grain size were observed by SEM images analysis. The electrical properties like variation of capacitance and impedance with different frequencies at room temperature were analysed from LCR meter instrument of both the samples.

d0020

Transient Eddy Current Oscillations Differential Probe to Detect Thickness of a Steel Plate

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Stainless steel structures like pipelines industries suffer from degradation due to aging and continuous usage in harsh environment conditions; this causes corrosion and local wall tinning which may initiate cracks. This change in wall thickness results in unwanted outages and catastrophic failures in structural materials. Thus regular inspection using Nondestructive Testing (NDT) techniques is mandatory to ensure the working and safe operation of plants. A Transient Eddy Current Oscillations (TECO) testing method has been employed for the detection of change in thickness in a steel plate. In the present study a differential probe has been is designed using two Hall-sensors to detect variation in thickness of SS304 specimen with different thicknesses varied from 1mm to 5 mm which is fabricated using with electro discharge machining (EDM) process. Different time domain features are extracted from the detected response from the probe and used to detect the defects having different depths in the test specimen.

d0021

Design and Development of High Temperature Seebeck Coefficient Measurement Set-up

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The paper presents a design and development of the temperature dependent (300-673 K) Seebeck measurement set-up for the bulk/thin films. The designed sample probe has compact structure with two copper blocks, mounted on a base plate with embedded ceramic heater. On one copper block an additional heater is mounted to generate a temperature gradient with respect to base heater. Both the heater has embedded K-type thermocouple to record temperature of cold end and hot end. To perform measurement in vacuum/inert atmosphere a SS chamber is designed to enclose the probe. For thermopower measurement, a temperature gradient (ΔT) is generated across a sample and thermo-emf (ΔV) is measured at temperature accuracy of ± 1°C, using Labview designed software. Test measurements are carried out on Cu and Ni rectangular block.

d0022

Increase in Hydrostatic Limit of Pressure Transmitting Medium Methanol -Ethanol with Temperature

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Methanol-Ethanol (4:1) mixture is the most widely used pressure-transmitting media in high-pressure diamond anvil cell based experiments. The quasi hydrostatic limit of PTM is nearly 10.5 GPa. In the article, we have investigated the hydrostatic limit of Methanol-Ethanol (4:1) mixture at 100 ^{0}C, 150 ^{0}C and 200 ^{0}C with ruby fluorescence technique using

internally heated diamond anvil cell. Our studies show that hydrostatic limit of the Methanol-Ethanol mixture can be extend up to 25±1.1 GPa by heating the mixture to 200 ^{0}C.

d0023

Evaluation Of Hydrogen Diffusion Parameters For Zr-2.5%Nb Alloy Pressure Tube Material using Neutron Radiography

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Abstract. Hydrogen embrittlement is a life limiting factor for Zr2.5%Nb alloy used in pressure tube of PHWR's. Reactor components during their lifetime pick up hydrogen produced as a byproduct of waterside corrosion. Hydrogen entering the metal matrix above the solid solubility limit precipitates as a brittle hydride phase ultimately degrading component performance. The hydrogen that enters the metal matrix is highly mobile and quickly redistributes itself under concentration, stress or temperature gradients leading to formation of hydride rims, blisters or delayed hydride cracking. Modeling of hydrogen diffusion requires prior knowledge of the various diffusion parameters. In this work we have evaluated hydrogen diffusion parameters for Zr-2.5%Nb alloy used as pressure tube material for Indian PHWR's using neutron imaging.

d0024

Monte-Carlo simulations of a high intensity – high resolution neutron diffraction instrument

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The installation of Advanced Materials Diffractometer (AMD) is scheduled to take place on beamline T1013 at the Dhruva reactor, BARC. This diffractometer will be replacing the current PD-2 diffractometer. The neutron flux at the sample can be expected to go up substantially and the best resolution can reach to 0.1% which will be 8 times better than the present PD-2 diffractometer. This instrument is envisaged to be world class, fostering new types of diffraction experiments. In addition to classical applications in high resolution powder diffraction this instrument can cater to time resolved diffraction studies with a time resolution of few minutes at slightly lower resolutions. To attain optimal performance of the optical components such as the monochromator and Söller collimators, Monte Carlo simulations were performed using MCSTAS, aiming to fine-tune their parameters.

d0025

The Introduction of Traps in Zinc Oxide Nanorods for the Development of Neuromorphic Memory Devices

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Structural defects in semiconductors are ambiguous and can act in either a damaging or beneficial role depending on the applications of the device. Neuromorphic devices require memory for operation, in such cases, trap centers for charge carriers can be created by defects and provide trap-related memory. Understanding and controlling defects are quite challenging to optimize device performance. This paper shows that the defect-induced trap states can be introduced in zinc oxide nanorods (ZnO NRs) during growth on the ITO-coated PET flexible substrate by seedless hydrothermal method in the presence of traces of surfactants. Utilizing X-ray diffraction, scanning electron microscopy, and photoluminescence spectroscopy (PL), the authors have analyzed the crystallinity, shape, and presence of defects in the growing ZnO NRs. Two different samples grown at different temperatures show different morphology with variations in trap states. PL study shows higher levels of trap states in 90ºC grown samples compared with 70ºC samples. This study suggests that trap states can be introduced by controlling growth parameters and by traces of surfactants. These traps in ZnO NRs can be beneficial for fabricating low-cost, multifunctional, transparent resistive random access memory (RRAM) devices for neurocomputing applications.

d0027

Structural, Microstructural and Raman Study of DyFeAsO

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Metal-based ceramic DyFeAsO has been prepared by well-known traditional solid-state reaction method. It is a special ceramic that is superconducting at low temperatures but acts as a semiconductor at high temperatures. We made structural, microstructural and Raman study to describe ceramics and their many applications. Crystal size and structural parameters are

found to be a=3.9086 Å, c=8.4575, Å, c/a=2.2201 which are determined at room temperature using X-ray diffraction (XRD) techniques. The surface morphology was examined by Field Effect Electron Microscopy (FESEM). Raman spectroscopy has been performed at room temperature in different frequency ranges from 100cm^{-1} and 2000cm^{-1}. W-H Plot gives the lattice strain which ensures the stability of the ceramic material.

d0028

Design and Deployment of Multi-axis Motion Control for Focusing Monochromator Assembly

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The upgradation of High-Q Diffractometer is scheduled to take place on beamline HS1019 at the Dhruva reactor, BARC. This diffractometer will be comprising of multiple resolution options with enhanced throughput. Soller collimator of 5' resolution will provide the best possible resolution at the instrument and the open geometry will correspond to highest flux. Addition of vertically focusing monochromator device is expected to enhance the monochromatic neutron flux by a factor of three. In addition to classical applications in high -q diffraction for amorphous materials, this instrument can cater to diffraction studies of disordered crystalline materials and corresponding Pair Distribution Analysis (PDF).

d0030

Tb(III) Activated Tungstate Phosphor for High-Energy Beta Radiation Dosimetry

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A tungstate double perovskite Ca_3WO_6 doped with 2.5 mol% of Tb^{3+} was prepared via combustion process using urea as a flux. The crystal structure identification of Ca_3WO_6:2.5 mol% Tb^{3+} phosphor was made by X-ray diffraction (XRD) pattern, and the monoclinic structure was discovered. A high-quality thermoluminescence (TL) was detected when phosphor was irradiated by high-energy beta rays. The effect of ionizing radiation dose and fading on TL intensity are the two major aspects studied in detail. The TL intensity demonstrated excellent linear response to the applied range of beta dose. The trap parameters of the studied phosphor were computed via the glow curve deconvolution (GCD). The fading effect on TL intensity was studied by recording the TL glow curves after one month of beta irradiation. Obtained results from the overall study shows that the phosphor under study have potential to be used in thermoluminescence dosimetry (TLD).

d0031

Investigating the Influence of Thin Film Thickness on Persistent Photoconductivity in β-Ga_2O_3 Photodetectors

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Gallium oxide shows potential for solar blind photodetection due to its 4.6 – 4.9 eV bandgap, ensuring solar blindness. Despite good photoconductivity, device performance can suffer from oxygen-related defects and persistent photoconductivity (PPC). We explore how thin film thickness affects PPC in solar blind photodetectors. Using RF magnetron sputtering, we deposit β-Ga2O3 onto sapphire with varying thicknesses, and a gold electrode via thermal evaporation. Thinner films exhibit enhanced PPC due to oxygen-related defects. Device performance hinges on thin film quality, stoichiometry, and oxygen defect levels.

d0032

Electrical And Photo-sensing Properties Of n-ZnO/p-Si (111) Heterojunction And Persistent Conductivity

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n-ZnO/p-Si(111) heterojunction was fabricated using DC magnetron sputtering followed by oxidation in air. Formation of ZnO thin film on top of Si (111) substrate was confirmed by X-ray Diffraction. Current-Voltage (IV) characteristics taken in the dark indicated the formation of p-n junction. Transient in photo-conductivity and switching property of the heterojunction was tested for various incident radiations such as infrared (IR), Ultraviolet (UV) and Green radiations in the reverse bias condition. The heterojunction showed a good photoresponse, especially for UV and IR radiation (13.96 and 14.3). On switching off the radiation, persistent conductivity was observed, especially for UV radiation.

d0034

Electrothermal Modeling to Analysis and Estimate Accurate Thermopower Value

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The efficiency of thermoelectric materials (TE) is directly related with the Thermopower (α). A standard system/set-up is considered to measure α of a TE material. Accurate measurement requires dedicated and rigorous technique. Several system-parameters viz., thermal resistance, contact resistance, carrier concentration etc. are incorporated in measurement of temperature dependent α. Electrothermal model is employed to estimate precise value of α. The calculations have been performed by taking following assumptions: a) System/set-up is one dimensional, length of all elements is much larger than the width and thickness in the measurement set-up. Hence, it may be considered that heat and electric current will flow along the length of the elements in set-up. And b) Heat is conducted through the sample only through conduction process. These results highlight the importance of considering several factors, during the determination of α for a TE material. It also emphasizes the importance of accounting the thermal resistance for accurate measurements.

d0035

A Novel Semiconducting Supramolecular Mg(II)-Metallohydrogel Based Resistive Random Access Memory Device With Excellent Endurance

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Supramolecular gels represent as a "smart" material which are used in many fields such as sensor, nanoelectronics, logic gate, memory device, cosmetics, environmental remediation etc. These gels are formed through the combination of hydrogels and supramolecular chemistry. In this work, we have prepared Mg(II)-ion based supramolecular metallohydrogel (i.e.Mg@5AP) by using 5-amino-1-pentanol in water at room temperature. Here, we have investigated the microstructural features of Mg@5AP from Field-emission scanning electron microscopy (FESEM). Furthermore, we have fabricated (Mg@5AP)-based planner device in a lateral metal-semiconductor-metal configuration to explore its charge transport behaviour. In this study, Mg@5AP metallogel based RRAM (Resistive random-access memory) device have showed a proper bipolar resistive switching behaviour at room temperature. This RRAM device demonstrated exceptional switching endurance with ON/OFF ratio of 100 upto 1000 consecutive switching cycles. Due to its enhanced stability, these structures are preferable for applications in non-volatile memory device, flexible electronics, and optoelectronics devices.

d0036

Automated Removal of Eyeblink Artifacts from Electroencephalogram in Heart Rate Variability Biofeedback Training Using Ensemble Empirical Mode Decomposition and Signal Space Projection

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The presented study introduces a novel approach for addressing the challenge of eyeblink artifacts in Heart Rate Variability Biofeedback (HRV-BF) training involving electroencephalography (EEG) data. Eyeblink artifacts can distort the EEG signal and impact the accuracy of data analysis. The proposed method combines Ensemble Empirical Mode Decomposition (EEMD) and Signal Space Projection (SSP) techniques to automatically detect and remove these artifacts from contaminated EEG data. EEMD adaptively decomposes non-stationary EEG signals into intrinsic oscillatory modes (IMFs), overcoming the mode mixing effect through the addition of identically distributed white noise. The methodology is validated using EEG data from a visual attention task, where eyeblink artifacts were detected and removed from the EEG recordings. The results demonstrate the effectiveness of the proposed method in minimizing distortion to the underlying brain signals, thereby improving data quality. This approach holds promise for scenarios where traditional artifact removal techniques are challenging to implement, such as in Magnetoencephalography (MEG) recordings where additional noise sources are a concern. Overall, this research contributes to enhancing the reliability of EEG data analysis in the context of HRV-BF training and similar applications.

d0037

Experimental Set-up of Magneto Optic Kerr Effect (MOKE)

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An in-house magneto optic kerr effect (MOKE) measurement set up has been designed to study the magnetic characteristics of different compounds. The set up consists of a laser source, polarizer, an analyzer, an electromagnet, a photo-elastic modulator (PEM), a lock-in amplifier and a LABVIEW program to facilitate the measurement. This MOKE set up was used to study the field dependent magnetization behaviour of YIG-based thin films and the results were compared with the vibrating sample magnetometer (VSM) measurements. The behaviour of the M-H loop is in agreement with the results obtained through the VSM technique. This evidently verifies the working of our set up.

d0040

Setting up a micro-Kelvin Laboratory at Bhabha Atomic Research Center, Mumbai

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Micro-Kelvin refrigerators play a crucial role in scientific research and technological advancements that require extremely low temperatures. This article discusses the ongoing relocation of an adiabatic nuclear demagnetization facility at Bhabha Atomic Research Center, Mumbai from Tata Institute of Fundamental Research, Mumbai. For reaching up to micro-Kelvin temperature this facility uses a high-power dilution refrigerator connected to a 5 kg copper stage through a superconducting heat switch. Various thermometry techniques are employed to measure temperature in different ranges. The expectation is to achievement temperature in the hundreds of micro-Kelvin range using this system. Achieving such low temperatures would enable researchers to explore and comprehend quantum phenomena and condensed matter physics.

d0041

Dependence of Second Pulse in IFNMR

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We have used a wide range of ferro/ferrimagnetic materials to study the response of these materials as a function of second pulse. Using the results of experiments, rather than the typical spin echo sequence, we discovered that samples with inhomogeneous broadening in the hyperfine field showed the strongest echo signal when exposed to two pulses of equal width. However, the normal spin echo sequence displays greater echo amplitude for the carbonyl iron and carbon coated iron samples with less hyperfine field broadening.

d0042

Investigation of Room Temperature NO_2 Gas Sensing Using WS_2 Nanoworms Deposited on Porous Silicon Substrate

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In this study, we present the room temperature sensing capabilities of a tungsten disulfide (WS_2) thin film for detecting NO_2 gas. The thin film was deposited onto a porous silicon substrate and the sensor was fabricated using DC magnetron sputtering on an anodized porous silicon base. Various characterizations, including X-ray diffraction (XRD), FE-SEM, EDX, and X-ray photoelectron spectroscopy (XPS), were employed to investigate the sample's phase, microstructure, atomic composition, and elemental bonding. The superhydrophobic nature of the fabricated thin film was confirmed using the sessile drop water contact angle method. Our proposed chemiresistive NO_2 gas sensor exhibited remarkable attributes such as strong responsiveness, an extensive detection range, high selectivity, and the ability to operate at room temperature. The outstanding sensing characteristics of the sensor are thought to arise from the combined catalytic properties of WS_2 and the expanded surface area due to the porous substrate, offering numerous adsorption sites.

d0044

Undulator-Based AMOS Beamline (BL-05) at Indus-2 Synchrotron Source: A Pathway to Probing Electronic Properties of Materials

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Vacuum ultraviolet (VUV) and soft X-ray spectroscopy have emerged as indispensable techniques for probing the intricate electronic behaviors in basic atoms and molecules to complex substances, even under extreme conditions. In this context, we introduce the planar permanent magnet (PPM) Undulator-based Atomic Molecular and Optical Sciences (AMOS) beamline (BL-05), recently commissioned at the Indus-2 synchrotron radiation source, RRCAT, Indore. This state-of-the-art experimental facility, specifically designed for VUV and soft X-ray spectroscopy, provides a powerful platform for exploring the electronic properties of materials in both gaseous and condensed phases.

d0045

Optimization of critical parameters of IFNMR

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Abstract: We studied radiofrequency (RF) power variation and, delay time dependence using a wide range of ferro/ferrimagnetic materials. Experimental observations optimized these parameters. According to experiments, RF power variation studies show that domain walls enhance more than domains at lower RF powers. The study also shows that soft

ferrimagnetic materials respond better to rf than hard ones. Further, the delay time dependence shows that all ferri/ferromagnetic samples relax quickly.

e) Single crystals, glasses and amorphous systems

e0001

Structure and Absorption Property of Nd (0.5 at.%) Doped $GdVO_4$ and $LuVO_4$ Single Crystal: A Comparative Analysis

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Single crystals of 0.5 at.% Nd doped $GdVO_4$ and $LuVO_4$ were grown by optical floating zone technique in a growth ambience containing 10 % oxygen. Structural parameters as well as other optical properties such as absorption coefficient and optical band-gap of both the crystals were evaluated and compared. The absorption coefficient of Nd doped $LuVO_4$ at 808 nm (8.2 cm^{-1}) and 880 nm (2.6 cm^{-1}) was found to be higher than that of Nd doped $GdVO_4$ (4.6 cm^{-1} at 808 nm and 1.9 cm^{-1} at 880 nm). The higher absorption coefficient is favorable for its use as laser gain medium. The band gap of Nd doped $GdVO_4$ and $LuVO_4$ was found to be nearly same. The estimated Urbach energy was ~80-85 meV for both the crystals, which was independent of host.

e0002

Enhancement of Eu^{3+} luminescence in Eu^{3+}/Ag Nano-particles Co-doped Boro-phosphate Glasses

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Eu^{3+}/Ag nanoparticles (NPs) co-doped borophosphate glasses have been prepared by conventional melt quenching technique and subjected to XRD, HR-TEM, absorption, luminescence and decay measurements. The presence of spherical Ag NPs inside the glass matrix was confirmed through the TEM analysis. From the absorption spectra, the bonding nature of the chemical bond between $Eu3^+$ ions and its ligand oxygen has been identified. The emission spectra were used to analyze the luminescence enhancement by Surface Plasmon Resonance (SPR) effect of Ag NPs and characterized by the CIE 1931 diagram to examine the dominant emission color. The decay curves exhibit single exponential behavior for all the studied glass irrespective of change in Ag concentrations.

e0004

Synthesis, Growth, Optical, Laser damage threshold Investigation of organic Piperazinium bis (P-aminobenzoate) dihydrate single crystal for Nonlinear Optical Applications

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Abstract. The organic single crystal Piperazinium bis (4-aminobenzoate) dihydrate (PPABD) was successfully grown through the slow evaporation solution growth method. Several characterizations were done in the PPABD crystal such as structural, optical, thermal, dielectric and NLO properties. The structural information was investigated by Single crystal x-ray diffraction (SXRD), SXRD results demonstrate that PPABD material belongs to the monoclinic system with non-centrosymmetric space group P21/n. According to a UV-Vis-NIR, the PPABD crystal has a large transmission window with a low near-UV cutoff wavelength of 327 nm. The LDT analysis was investigated by ND: YAG laser and the wavelength of laser is 1064 nm. The open aperture z-scan technique was used to investigate the NLO absorption of the sample at 632.8 nm.

e0005

Novel metal-organic framework and crystal engineering of Bismorpholinium mercury (II) tribromo chloride (BMMC) for optoelectronic applications

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A novel metal-organic non-linear optical crystal, Bismorpholinium mercury (II) tetrabromide (BMMC), has been synthesised, and optically transparent single crystals have been successfully grown by slow evaporation solution growth technique (SEST). The formation of the new crystalline structure and the morphology of the grown crystal were determined using single-crystal X-ray diffraction (SXRD) analysis. The BMMC material crystallises in a monoclinic crystal system with the space group of $P2_1/c$. The unit cell has four molecules accumulated in it (the unit cell parameters are a = 6.8056(6) Å, b = 14.0027(10) Å, c = 17.2152(14) Å, β = 93.148 (3)°and Z=4The BMMB single crystal with a thickness of 2 mm shows a good optical transmittance of about 75% in the visible and NIR regions with a cut-off wavelength of 328 nm. The crucial thermal parameters such as thermal stability, decomposition point and the melting point of the BMMC single crystal have been determined using Thermogravimetric (TG) and Differential thermal analysis (DTA) under a nitrogen atmosphere. Third-order non-linearity of the BMMC crystal has been evaluated by open and closed aperture Z-scan measurements using Nd: YAG laser at 532 nm.

e0006

Growth of (001) Plane of 2-Ethylimidazolium D-Tartrate Single Crystal and Study of Its Optical Properties for NLO Applications

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A potential organic single crystal of 2-Ethylimidazolium D-Tartrate was grown in the (001) direction using Sankaranarayanan-Ramasamy (SR) method. The transmission of the harvested SR crystal is more than 80% in the range of 400 to 800 nm. The in-plane refractive index was measured by prism coupling technique. It is observed that as the wavelength increased, the refractive index decreased. Third order NLO properties were scrutinized using Z-scan method. The calculated third order susceptibility value is 1.7 × 10^{-9} esu.

e0007

Transport Properties of Mn and S Doped Bi_2Se_3 Topological Insulator

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The transport properties of Mn and S co-doped Bi_2Se_3 topological insulators have been investigated in the present work. The X-ray diffraction pattern indicates the single crystallinity of the sample. The resistivity behavior clearly shows the metallic nature,which indicates the existence of surface state. The magneto-transport behavior and Landau level indexing confirms the topological state in the sample.

e0008

Characterization of Lead Silicate Glasses for Radiation Shielding Application

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We report detailed studies on synthesis and characterization of CeO_2-BaO-PbO-K_2O-B_2O_3-SiO_2 glass systems for possible radiation shielding window application. Glass composition was optimized by varying the components and density of 4.5 gm/cc was achieved. The half value layer thickness was measured as 3.2 cm from Co-60 gamma. No drastic changes were measured in HVL post gamma irradiation. Glass doped with 1wt% of CeO2 showed best radiation resistance against browning up to 100 kGy doses in gamma chamber. No changes in transmission with different dose rates for absorbed dose of 1kGy were observed. The structure-property correlation after exposure to gamma irradiation was evaluated to understand the post irradiation changes in this glass system.

e0009

Physical and Optical Insights of Holmium Doped Borate Glass for Optimization of Efficient Laser System and Luminescent Devices

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Borate glass doped with Holmium (Ho^{3+}) having different concentration were synthesized via melt quenching method. Physical properties including Density (ρ), Molar volume (V_m), Crystalline volume (V_c), Interionic distance (R_i), Field strength (F), Polaron radius (R_p), Oxygen packing density (OPD), Refractive index (n), Molecular electronic polarizability (α_m), Reflection loss (R_L), Transmission coefficient (T), Dielectric constant (ε), Metallization (M), Molar refractivity (R_m), Optical electronegativity (χ_{opt}), and Optical dielectric constant (ε_{opt}) were investigated with the variation of the concentration of Ho^{3+} ions. Absorption spectra was recorded in range of 200nm-1500nm and eight peaks are observed. Using the Davis and Mott relation, both indirect and direct optical band gap (E_g^{opt}) were calculated. Further, the as-prepared glasses possess the electrical characteristics that are explained by the Urbach energy (ΔE) determined from the absorption spectrum. The known result affirm the glasses potential in green luminescent devices as well as a green component in white LED fabrications.

e00010

Translational And Rotational decoupling of relaxation dynamics in a Supercooled binary mixture

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We present a study of translation and rotational(reorientation) dynamics of a binary mixture of FENE dumbbell molecular liquid and monatomic molecule where the non-bonding interatomic potential is that of a well-known glass-forming binary

mixture. In the extended model of the glass forming system with rotational motion, we find many signatures of glass transition, such as dramatic slow down of density relaxation, decoupling of the translational and rotational relaxation, etc. A comparison of variations in the signature of glass transition at higher and lower densities shows that translational-rotational decoupling at lower density is more due to the formation of cavities that enhances surface mobility, which increases the dynamic heterogeneity.

e00011

Indian natural monazite: Elemental identification and analysis of structural properties

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The present work discusses the effect of various radioactive and non-radioactive impurities present in the natural monazite crystalline sand powders on the crystalline and their vibrational properties have been discussed in the present work. Monazite sample was obtained from the IREL (India) Limited for the beneficiation of the society. TXRF measurements were performed to using synchrotron radiation to determine the details of various impurity elements present in the sample, which revealed the presence of Ce, La, Nd, Pr, Ca and Fe as the major elements, while the presence of U and Th in trace amount was also seen. Synchrotron radiation based XRD measurements showed the crystalline nature of the sample. In contrast to the previous reports, Raman spectroscopic measurement exhibited modified relative intensities of different vibrational peaks compared to earlier work, which may be correlated with the possible fluorescence (Photoluminescence) of the sample, which arises from the presence of radioactive impurities like U and Th.

e00013

Effect of Silicate Units on Optical and Structural Properties for Various Automotive Windshield Glasses

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The Windshield glasses of Maruti Alto 800 (A800), Hyundai i20 (Hi20), and Maruti Suzuki Eeco (MSE) are taken from an automotive repair shop for investigating their structural and optical properties to check their durability. Fourier transform infrared (FTIR) was used to study the fundamental mode of vibrations and structural units present in available windshield glasses. The UV- visible spectroscopy was used to determine the transparency of these windshield glasses. It is found that the structure of glass A800 is highly polymerized due to the presence of the most prominent Q^2 unit and constant transparency throughout the variable range.

e00014

Growth and Characterization of NLO Active Sodium Substituted Potassium P-nitrophenolate Dihydrate (Na-NPK.2H$_2$O) Single Crystal

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A new initiative has been taken to grow single crystals of sodium-substituted potassium p-nitrophenolate dihydrate (Na-NPK.2H$_2$O) in methanol for the first time. The single crystal X-ray diffraction investigation of Na-NPK.2H$_2$O revealed the crystal to be monoclinic with a non-centrosymmetric space group of $P2_1$.The UV-visible spectrum of the crystal exhibited enhanced optical properties with the synergetic presence of sodium and potassium. The sharp broad emission peak at 526 nm in the photoluminescence spectrum indicated green emission. In the FTIR analysis, functional groups of sodium and potassium metals were found with their corresponding peaks. The thermal studies revealed the crystals to be stable up to 127 °C. Thus the combined effect of sodium substituted potassium para-nitrophenolate dihydrate single crystal could effectively be employed in opto-electronic devices and nonlinear optical applications.

e00015

Exploring the Influence of Natural Dye on the Optical, Thermal and Nonlinear Optical Behavior of a Lithium Paranitrophenolate Trihydrate Single Crystal

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Dye embedded crystals gain a lot of interest and attention in solid-state and nonlinear optical applications. In the present work, a novel way of incorporating natural dye in LiPNP single crystal has been explored. With the insertion of *Clitoria Ternatea*

(CT) dye extract as dopant, a new attempt is made to enhance the growth rate, optical, thermal and nonlinear optical properties of LiPNP single crystals. The pure and CT doped LiPNP (CT-LiPNP) grown crystals exhibited differences in their colour and growth period. The organic functional groups in the FTIR spectra of dye-doped crystals with shifted peaks served as further confirmation of this alteration. Clear variations in the cut-off wavelength and emission spectra were observed for pure and CT-LiPNP crystal through UV-Visible and Photoluminescence spectra analysis. The decomposition temperature of the CT-LiPNP crystal was found to be high when compared to the pure LiPNP. The SHG test confirmed that CT-LiPNP crystal has enhanced efficiency which is 2 times higher than that of pure LiPNP. Therefore, natural dye-doped crystals could unlock the door to entirely novel optoelectronic device applications.

e00016

Investigation on the role of crystal thickness on wavelength tuning in optically pumped Amplified Stimulated Emission

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Since the discovery of laser, organic fluorescent materials have been favoured by most of the researchers due to their high photo-luminescence quantum yield (PLQY), easy and low cost crystal growth/thin-film fabrication and possibility to develop bio-friendly devices. Particularly, Organic single crystals (OSCs) with long range crystalline order, almost parallel crystal facets and high refractive index is highly preferred, as they give rise to inherent Fabry-Perrot resonator cavity for light amplification. So with a minimal setup and creative strategies to adjust the physical dimensions of the single crystal, the Amplified stimulated emission (ASE) can be tuned. To be specific, the thickness of the material has a direct impact on the emission wavelength of the ASE In the present work, we have demonstrated the crystal thickness dependent wavelength tuning in two well-known thiophene/phenylene derivatives. It has been observed that with a proper choice of crystal thickness it is possible to tune the emission upto 20 nm in the case of BP2T and upto 40 nm in the case of BP3T.

e00017

Fast Neutron Detection Capability of a High Dye Loaded Polystyrene Based Plastic Scintillator

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This report discusses the fabrication of an advanced clear and transparent plastic scintillator with high dye concentrations through bulk thermal polymerization. The scintillator consists of a styrene base matrix mixed with two dyes: 2,5-diphenyloxazole (PPO) with UV emission and 3-hydroxyflavone (3HF) with emission at 530 nm. The addition of 3HF prevents self-absorption, improving energy transfer efficiency between the dyes. The scintillator demonstrated good performance for fast neutron detection, with maximum emission at 540 nm and fast scintillation decay under neutron and gamma excitation. An effective neutron/gamma pulse shape discrimination with FOM of 1.6 and excellent energy linearity are exhibited.

e00018

Humidity Sensing studies on Binary Bismuth Borate Glass and ZnO-Glass Heterostructures

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Semiconducting bismuth borate glass and ZnO-glass heterostructure samples are studied for humidity sensing. Glasses in the composition of $0.5Bi_2O3–0.5B_2O_3$ are obtained by melt-quenching process, whereas ZnO prepared by sol-gel method. ZnO-glass heterostructure samples are obtained by adding pulverized glass powders in different weight fractions to the ZnO sol-gel solution. Heterostructure thin-films are deposited by drop casting method on the Si and flexible paper substrates. Structural and microstructural characteristics of the samples are studied using X-ray powder diffraction (XRD), and scanning electron microscope (SEM). ZnO and ZnO-glass heterostructure samples are tested for humidity sensing at room temperature by monitering change the resistance of the samples. Pure glass and ZnO-glass heterostructures at high glass concentration have shown high sensitivity factors to humidity than pure ZnO. Further, humidity sensing of the samples on flexible paper substrates are carried out and results are discussed.

e00019

Effect of Minority Composition in a Binary Glass Forming Liquids

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The glass transition of Lennard-Jones particles is a fascinating phenomenon that has been studied extensively in recent years.This study is performed using molecular simulation to understand the slowdown of relaxation process with varying concentration of minority particles in a binary glass forming liquids. As concentration of minority particles is increased, these systems start to show correlation between local density or cage density and slowdown of relaxation time. We show that with

increase of the impurity concentration the local density at which divergence of dynamics decreases with increase in concentration of impurity.

e00020

Relation Between Local Density Debye-Waller Factor and Density Relaxation during Glass Transition in Model Systems

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This molecular dynamic simulation study of a glass-forming binary mixture and FENE polymer sheds light on the structural origin of slow relaxation in these two glass formers. We show that the growth of the highest peak of the radial distribution function g(r), and variation in density relaxation, are correlated, which is related to the free volume available for density relaxation in the free volume theory; we also compare the growth of the surface density at the first peak to the Debye-Waller factor, which is also a representation of free volume is connected to the local density by a power law in the moderately supercooled regime in these two different systems.

e00021

Ion-beam impact in zirconolite ceramic compositions

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Despite being a clear, safe and reliable source for generation of electricity, nuclear energy has major drawbacks due to the production of high-level wastes (HLW) releasing harmful radiations. Zirconolite, a prospective candidate for immobilization of nuclear wastes has been studied to investigate radiation damage behavior under the induced effects of electronic energy loss. Zirconolite compositions, $CaZrTi_2O_7$ and $Ca_{0.8}Nd_{0.2}ZrTi_{1.8}Al_{0.2}O_7$ prepared using two-step solid-state sintering method were irradiated by 120 MeV Au^+ ions and 30 keV He^+ ions. Under swift heavy ions, XRD studies showed loss in crystallinity and lattice contraction of samples with increasing ion fluence. Further, both compositions amorphized at high fluence of 3×10^{13} ions/cm^2 with some residual diffraction peaks. The approach of amorphization followed the single ion impact model. He^+ ions with 30 keV energy impacted the crystallinity of the zirconolite by inducing strain through the formation of dislocation loops and accumulation of He bubbles. No sign of amorphization was observed through XRD under the effects of light He^+ ions. Though, significant surface damage and redox behavior was seen for both compositions at 1×10^{17} ions/cm^2 from XPS study.

e00022

Bulk Synthesis and Crystallization of 2-methylimidazolium based Manganese(II)halide Complex {($C_4N_2H_7$)[$MnCl_3(H_2O)$]$_n$}: A Red Luminescent Material

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This work aims to describe the bulk and eco-friendly synthesis of luminescent manganese (II) complexes possessing $[Mn(X)_6]$ anionic octahedral chains, with 2-methylimidzole counter cations for various technological applications. The present method envisages that the exposure of acidic vapors on the precursors itself could lead to the bulk synthesis of the materials, and may possibly replace the time consuming crystallization attempts. The title complex, which is originally synthesized from the crystallization method is chosen as a test case to validate the hypothesis. In the present study, bulk synthesis was achieved by exposing the solid mixture of manganese (II) acetate (metal ion source) and 2-methylimidazole (organic moiety) to the HCl vapor in a closed environment. The product was directly obtained as a microcrystalline powder and the structural identity was confirmed by powder X-ray diffraction and FTIR methods. This research work provides a new and efficient strategy for bulk synthesis of the 2-methylimidazolium tetrachloromanganate(II) complex.

e00023

Synthesis, Growth, and Characterization of Inorganic-Organic Hybrid Material: Tetrabromo Bis (2-Amino-4-Methyl the Pyridinium) Zincate (II)

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Single crystals of inorganic-organic hybrid material, tetrabromo bis (2-amino-4-methylpyridinium) zincate (II) (TB2A4MPZ) have been investigated. A transparent single crystal is grown by slow evaporation solution growth method using water as a solvent. The crystal structure has been determined by single-crystal X-ray diffractions study and it crystallizes in the triclinic crystal system with centrosymmetric space group P-1. The structure of the title compound is built from isolated [ZnBr4]2- anions and [2-amino-5-methylpyridinium]+ cations which are connected through N-H•••Br hydrogen bonds. The infrared spectrum proves the presence of the functional group in the synthesized compound. The UV-Vis-NIR study shows that grown crystal has good transparency in the wavelength region of 230-1100 nm. The grown crystal was characterized thermally by carrying out thermo gravimetric measurements and it is found to be stable up to 146 ºC

e00024

Titanium-Tungsten Oxide Doped Borosilicate Glasses for Near- Infrared -Shielding Borosilicate Glasses for Energy - Saving Applications

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NIR-shielding glasses were synthesised by direct embedding of Ti-WO_{3-x} in borosilicate glass during a facile melt-quenching process. The distribution of Ti-WO_{3-x} functional unit in the glass was confirmed by sample characterization using XRD, SEM and EDS. The NIR-shielding property has been attributed to local surface plasmon resonance due to oxygen vacancies in the Ti-WO_{3-x}functional unit. Optical performance measurement using UV-Vis-NIR spectrophotometer is under investigation. This study sheds a light on fabricating energy-saving windows with a tunable NIR-shielding performance.

e00025

Influence of Cobalt Ions on Spectroscopic and Emission Characteristics of Lead Aluminia Bismuth Phosphate Glass System

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By using the conventional melt quenching method, PbO-Al_2O_3-Bi_2O_3-P_2O_5 glasses doped with varying concentration of CoO were prepared and characterized. The optical absorption spectra of the glasses exhibited two principal absorption bands, one at 572 nm and the second one consisting of multiplets with the meta centre around1487 nm ascribed to thetetrahedrally coordinated Co^{2+} ions. Besides these, the spectra also exhibited two feeble bands around 532 and 633 nm which are the characteristics of octahedral coordinated Co^{2+} and Co^{3+} ions, respectively. Photoluminescence spectra of the titled glasses have exhibited two emission bands at 640 and 868 nm due to tetrahedral Co^{2+} ions. FTIR spectra of the samples exhibited various vibrational bands due to phosphate, bismuth, PbO_4, PbO_6, AlO_6, AlO_4 and Co^{III}-O vibrational units. The studies on the titled glasses have revealed that tetrahedrally coordinated Co^{2+} ions are found to increase as the content of CoO is gradually increased up to 0.8 mol%. As a result the degree of depolymerization of the glass network decreases which in turn enhances its rigidity with increasing the concentration of CoO upto 0.8mol%.

e00026

Understanding the nature of neutral, charge assisted and deuterated O-H—O hydrogen bonds using structures extracted from Cambridge structural database

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One of the most common class of hydrogen bond found in molecular crystals is the O-H---O hydrogen bond, these can be is neutral $(O\text{-}H\text{---}O)_{neutral}$, negatively charge assisted O-H---O^- or positively charge assisted O^+-H---O . Utilizing the Cambridge structural database we have extracted structural information regarding the different types of O-H—O hydrogen bonds and statistically analyzed the information to get some insight into the general nature of the O-H---O hydrogen bonds. It is found the nearly 90% of O-H---O all hydrogen bonds exhibit electrostatic behaviour about 10% exhibit weak dispersive behaviour, where as hydrogen bonds belonging to covalent category are rare. The most important observation obtained from this data analysis is that there are no deuterium bonds (O-D---O) belonging to the covalent category, reasons and consequences of this observation is discussed.

e00027

The Diethyl Oxalate And N-Methyl Acetamide Crystallization Leading To Oxalic Acid Dihydrate Crystals

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The crystallization is a result of interplay of intermolecular interaction between the initial components which are used to form cocrystal or compounds. Diethyl oxalate and N-methyl acteamide exists as liquid at room temperature. The mixing of two liquids in their equimolar ratio at room temperature resulted in the formation of oxalic acid dihydrate crystals, which was characterized by single crystal X-ray diffraction. The formation of oxalic acid dihydrate can be explained as hydrolysis of diethyl oxalate in the presence of N-methyl acetamide as catalyst at room temperature.

e00028

Theoretical Formulation Glasses Specific Heat: A Breach of Dulong & Petit Law at High Temperature

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Given the lack of theory, it is long standing problem to comprehend the specific heat of glasses at both high and low temperatures. At the glass transition (Tg), glasses exhibit structural relaxation. We are claiming that the Dulong and Petit laws are broken by the specific heat of solid glasses created from frozen liquid from the melt T<Tg and T<Tm liquids state (below melting) it is due to the presence of floppy modes affect the internal energy. This article attempts to solve the riddle of glass. Ge15Se85, Ge20Se80, and Ge25Se75 measurements were made using modulated differential scanning calorimetry (MDSC). At high temperatures, the specific heat of glasses is regarded as a step potential function. When liquid reaches the glass transition temperature, it becomes more viscous and exhibits a leap in specific heat. Despite being a second order kinetic phase transition, the glass transition's specific heat shows a boost because the glass goes from a frozen liquid to a more viscous liquid. In terms of the variation of power exponents, we conducted analysis on the specific heat of glasses with compositions in the ΔCP area. Data have been analyzed for ΔCP and configurational entropy SC across compositions which is also a measure of glass fragility; at the Kauzmaan temperature (TK) configurational entropy equals to zero.

e00029

Effect of Co doping in Bi_2Se_3 topological insulator: probed by XRD, ARPES and EXAFS

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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. Here we report a systematic study of the local structural environment in Co doped Bi_2Se_3 single crystals grown by vertical Bridgman technique using X-ray diffraction (XRD), Angle resolved photo electron spectroscopy (ARPES) and X-ray absorption fine structure (XAFS) measurements.

e00030

Solving the problem of Cracking in $CeBr_3$ Single Crystal in Bridgman Technique

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The growth of $CeBr_3$ single crystals poses challenges due to their hygroscopic and highly crack-prone nature. These issues have been addressed by incorporating aliovalent dopants such as Ca, Ba, and Sr into $CeBr_3$. Among these dopants, Ba has proven particularly effective in reducing the crystal's propensity for cracking and its hygroscopic behavior. Furthermore, we successfully resolved the vertical cracking problem in the growth of 1-inch diameter single crystal of $CeBr_3$ by implementing crucible rotation during the cooling cycle.

e00031

Growth of $Cd_{0.92}Mn_{0.08}Te$ single crystal for application in room temperature gamma-ray detection

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In this report, growth of $Cd_{0.92}Mn_{0.08}Te$ single crystal by modified vertical Bridgman technique is discussed. Single crystalline nature was confirmed by the Laue diffraction and zinc blende crystal structure with lattice constant 6.4766Å was found using powder X-ray diffraction analysis. The bandgap (1.5020 eV) was estimated using NIR spectroscopy. A higher transmittance of over 60% is observed in the FTIR transmittance measurement. Tellurium inclusions and their size were determined by infrared microscopy. The detector's resistivity determined by I-V is ~ $1x10^9$ Ω.cm. Energy resolution at 59.5 keV of ^{241}Am gamma source is ~22.8%.

e00032

Growth of optically transparent trans-stilbene single crystal by modified vertical Bridgeman technique for neutron and gamma-ray detection applications

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In this paper, we have investigated the growth of large-sized trans-stilbene (TSB) single crystal using the modified vertical Bridgeman technique (VBT). The optimization of the parameters such as furnace setup, ampoule's cone angle, and material purification were mainly focused during the growth process. The emission wavelength at visible region, the fast scintillation decay and the PSD properties marks its significance in scintillator detector applications.

e00033

Tailoring Optical and Structural Properties of $LaCl_3$ Single Crystals through Sr Doping: An Extensive Investigation

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$LaCl_3$ is well known single-crystal scintillators for the detection of fast neutrons and gamma. To see the effect of Sr doping on the performance characteristics of $LaCl_3$ single crystals, single crystals doped with Sr were grown with optimized growth rate in 4 zone Bridgman furnace. To investigate the effect of Sr doping on crystal properties, radio luminescence, thermo luminescence, and scintillation properties were studied in details.

e00034

Effect of Temperature Gradient on the Single Crystal Growth of Ti-Sapphire Single Crystals

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Ti^{3+} doped Sapphire is known for its exceptional optical properties, particularly in the realm of laser technology and is widely used as tunable solid-state lasers and optical waveguides. However, maintaining a uniform concentration for the Ti3+ ion along the grown crystal is a challenge and the temperature gradient and crystal growth parameters plays an important role in the optical quality and the defects generated during the growth. We report the single crystal growth of 0.2 mol % Ti doped Sapphire and the related challenges in the growth and the titanium distribution along the crystal. We are discussing the optimization of some of the crystal growth parameters used in this study to address these challenges.

e00035

Influence of Er^{3+} on Optical Properties of Bismuth-based Lithium Borate Glasses

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Borate glasses are well known to be a potential candidate for optical fibre amplifier applications. The present study focuses on the optical properties of $30Li_2O+60B_2O_3+(10-x)BiCl_3+ x\ Er_2O_3$ (x = 0,…. 3 mol %) glass systems. The glasses were prepared using the conventional melt-quenching method. XRD patterns confirmed the amorphous nature of the glasses. Band gap energy and Urbach energy were determined using diffuse reflectance spectroscopy and found to be in the range of 3.03 eV to 3.33 eV and 0.47 eV to 1.36 eV respectively. The values of the refractive index, calculated from the experimentally determined band gap energy values were found to increase (2.38 to 2.30) with the increase of Er_2O_3 content in the glass system. The vibrational modes corresponding to the structural units present in the glass system are explored using infrared spectroscopy.

e00036

Reaction Characteristics of Cesium Species with Fly Ash and Iron Pyrophosphate

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Two inorganic materials viz., fly ash and iron pyrophosphate were examined for trapping of cesium vapour species at elevated temperatures. Adsorbents in the form of porous pellet or filter were used for the absorption of cesium vapour. Various techniques such as XRD, Raman, Infrared and SEM were deployed for characterizing cesium exposed fly ash and iron pyrophosphate. Cesium vapour species reacted with fly ash and formed stable nepheline and pollucite phases. The reactivity of cesium vapour towards iron pyrophosphate was not clear and XRD data suggested the formation of $CsFeP_2O_7$ as a minor phase.

e00037

Reverse Monte Carlo Modelling of neutron diffraction data from 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 property of these glasses. Obtained pair distribution functions for P–O and Fe–O bonds showed a notable change at 20 mol% modifier concentration.

e00038

Understanding the Local Structure and Network Connectivity of Cerium Tellurite Glasses through Neutron Diffraction

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The structure of Cerium-Telluride glass systems has been studied using neutron diffraction technique. Analysis of diffraction data is done by using Reverse Monte Carlo modeling. 3D configurations have been built for all the glasses to understand the correlation between glass network. The short-range order and co-ordination number distribution has been successfully determined and have been compared as a function of Cerium Oxide concentration. We show that these systems have TeO4 bi-pyramidal, TeO3 trigonal pyramid and CeO6 polyhedral units as short-range order. The number of TeO3 structural units increases, thus decreasing the average Te co-ordination number, for glasses of higher CeO2 concentration.

e00039

Comparison of Two-Coil Pick-up Response of Kondo Insulator SmB_6 and Topological Insulator Bi_2Se_3

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Kondo insulator SmB_6 shows formation of a bulk Kondo insulating gap in the sample between 30-50 K, while conducting surface state characteristics appear only below 4 K. Here, we compare the two-coil mutual inductance pick-up response of SmB_6 to that of a conventional topological insulator, Bi_2Se_3, and identify three distinct temperature regimes for SmB_6, viz., (i) T □ T^*(~ 66 K), (ii) (40 K~) T_g □ $T < T^*$, and (iii) $T < T_g$. Across all these regimes, distinct T dependence and AC frequency dependence are observed. Results of our investigations suggest that above T^* weak exchange interactions cause electrons to scatter from random ion sites. Electronic correlations gradually strengthen below T^*, and at T_g, a bulk Kondo insulating gap starts to form. The appearance of a thin high conducting surface layer is nearly coincident with the onset of the bulk Kondo insulating state below T_g in SmB_6.

e00040

Comparison of Two-Coil Pick-up Response of Kondo Insulator SmB_6 and Topological Insulator Bi_2Se_3

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e00041

Role of Fe_2O_3 and MoO_3 content on FTIR study of Lead Borate Glasses

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Glasses with compositions xM.(40-x)PbO.60B_2O_3 (M = MoO_3 and Fe_2O_3) have been synthesized by the standard melt-quenching technique. The FTIR spectra were recorded in the wave number range of 400-1600cm^{-1} and three bands were observed in each glass sample. From the FTIR study, it was found that Fe_2O_3 containing borate glasses exhibit better absorption bands than the lead borate glasses containing MoO_3 content. Moreover, the intensity of all three bands of Fe_2O_3-doped lead borate glasses is higher than that of the corresponding MoO_3-doped bismuth borate glasses.

e00042

Structural, Thermal and Optical properties of Na_2O-CdO- GeO_2-SiO_2 Glasses doped with SeO_2

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25Na_2O-5CdO-(15-x) GeO_2-55SiO_2: SeO_2 (x = 2,4,6,8 and10 mol%) glass samples have been prepared by melt quenching technique. Glass phase of the samples was verified by XRD and DTA. The elemental content was confirmed by EDS. The

optical absorption spectra in the range of 300-1100 nm wavelength for the samples have been recorded. The E_g exhibited minimal value 2.369 eV for 10 mol % of SeO_2. Urbach energy ΔE is found to increase from S1 to S5. The FTIR spectra of the prepared samples provide the information about various structural units viz., Rocking vibrations of Si-O-Si structural units, bending modes of Ge-O-Ge bonds, vibrations of (Na^+), vibration of Se ions, Symmetric stretching vibration of Si-O-Si bands, asymmetric stretching vibration of $[SeO_3]^{2-}$ groups, and SiO4 units that are present in these glass matrix. It is observed that, with increasing the concentration of SeO_2 up to 10 mol% the intensity of above asymmetric and octahedral vibration modes increases at the expanse of symmetric and tetrahedral vibrational modes in the glass matrix indicating the relatively high semiconducting nature of S_5 sample.
Key words: Melt quenching; XRD, DTA, EDS and FTIR spectra.

e00043

THERMAL STABILITY AND PHYSICAL PARAMETERS OF Te(1-x)(GeSe0.5)Yx (x = 0, 0.05, 0.1, 0.15) CHALCOGENIDE GLASSY ALLOYS

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Differential scanning calorimetry (DSC) has been studied in the present work. DSC runs were performed on each sample at distinct heating rates (5, 10, 15 and 20K/min). The glass transition temperature (Tg) gives important information about the characteristics of materials such as thermal stability, glass-forming ability, and crystal growth kinetics. Activation energy has been computed by using Kissinger and Moynihan technique. $Te_{(1-x)}(GeSe_{0.5})Y_x$ glassy alloy thermal stability has also been determined by the Dietzal relation, Saad and Poulin relation, Hurby parameter (Hr), Lie and Liu parameter. The study of the compositional dependency of characteristics related to thermal stability has also been determined. The average coordination number and the total number of constraints for the $Te_{(1-x)}(GeSe_{0.5})Y_x$ (x= 0, 0.05, 0.1, 0.15) alloys have been addressed using two topological effects, floppy and rigid transition. To comprehend the structural characteristics of glasses, the chemical bond technique has been used to analyze mean bond energy and glass transition temperature. Theoretically, the glass transition temperature, mean bond energy, and heat of atomization have all been investigated.

e00044

Ge Single Crystal Growth: Simulation Studies On The Effect Of Rotation On Melt Flow And Thermal Gradient

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The Crystal growth simulation of germanium single crystal under hydrogen ambient by Czochralski crystal growth technique is carried out employing the COMSOL multiphysics software based on finite element analysis. Effect of crystal rotation on the thermal profile and melt flow conditions were modeled employing various approximations. It is shown that rotation rate changes the radial temperature profile at free melt surface. Also the forced convection introduced (~ 1-2 mm/s) by rotation breaks the natural convection flow making the flow rate more homogenous across the melt and completely reversing the flow direction at solid-melt interface.

e00045

Medium Range Order in a-MoGe Thin Films

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Structural characterization of amorphous solids is important due to its potential for engineering applications. Amorphous solids do not have a long range order as in crystalline solids, however, they exhibit a Medium Range Order (MRO), which may extend up to about a few nm length scale. Routine Electron Diffraction or x-ray Diffraction techniques are not sensitive to MRO. In a transmission electron microscope (TEM), statistical normalized variance of the speckle contrast (in dark field images) due to electrons scattered by a thin amorphous sample is used to calculate the MRO length scale.
We have used the variable resolution fluctuation electron microscopy (FEM) to calculate the MRO length scale in amorphous Molybdenum Germanium (MoGe) films of 5 nm and 20 nm thickness prepared by pulsed laser deposition (PLD). We found that the MRO length scale in the films with 20 nm and 5 nm thickness was 0.7 nm and 1.04 nm respectively.

e00046

Role of tungsten ions on the physical and spectroscopic properties of $Na_2O–PbO–Bi_2O_3–SiO_2$ multi-component glass system

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The Glasses under investigation were synthesized by melt quenching technique. Their XRD spectra confirmed the amorphous nature. These samples were spectrally analyzed by optical absorption, EPR and FTIR. The increase in the intensity of bands

in the optical absorption spectra and resonance signal in the EPR spectra of tungsten doped samples indicated the increasing order of W^{5+} ions at the expense of W^{6+} ions with the increasing concentration of WO_3. These W^{5+} ions occupy octahedral position and act as modifiers, causing the structural disorders leading to depolymerization in the glass network. The FTIR spectra of these samples exhibited the vibrational bands due to various structural units present in the glass network. The decrease in the optical band gap and increasing degree of disorder in the glass matrix result the decrease in the rigidity of the glass network which enhances the semiconducting character with increase in the concentration of WO_3. The results of various spectroscopic studies have indicated that titled glasses doped with 5 mol% of WO_3 are better candidates for exhibiting photochromism since they contain higher proportions of W^{5+} ions.

e00047

Structural Analysis of Zinc Phosphate Glasses Doped with Different Concentrations of Dy3+ Ions for WLED Applications

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In this study, the structural and optical properties of zinc phosphate (ZnP) glasses doped with different concentrations of Dy^{3+} ions in the (60-n)P_2O_5-20ZnO-10SrO-10LiF-nDy_2O_3composition were investigated. The glasses were prepared using the melt-quenching technique and characterized by X-ray diffraction, scanning emission microscope (SEM), Fourier transform infrared spectroscopy, and Raman spectroscopy and Photoluminescence spectra. The density of the glass increased linearly with the Dy^{3+} concentration. The amorphous nature of the ZnP glasses was confirmed using SEM analysis and XRD profiles. In addition, the presence of elements in the composition was confirmed using EDX. The FTIR spectra of the ZnP glasses exhibited vibrational bands matching the characteristic phosphate groups, which was further confirmed by Raman analysis. The emission spectra showed three prominent bands corresponding to the $^4F_{9/2} \rightarrow {}^6H_{15/2}$ (blue),$^4F_{9/2} \rightarrow {}^6H_{13/2}$ (yellow), and $^4F_{9/2} \rightarrow {}^6H_{11/2}$(red) transitions of the Dy^{3+} ions excited at a wavelength of 350 nm. The chromaticity colour coordinates, and correlated colour temperatures of the glasses lie in the cool white-light region.These results suggest that ZnP glasses doped with Dy^{3+} ions have potential applications as white light-emitting materials for solid-state lighting devices.

e00048

Structural and Luminescence Investigation on Eu^{3+} Doped Alkali Borophosphate Glasses for Photonic Applications

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The structural and luminescence properties of Eu^{3+} doped alkali boro-phosphate glasses for the potential applications in photonic devices are investigated. The fundamental stretching units of borate and phosphate are observed in the FTIR spectra. By using the absorption spectra, the bandgap energy and the urbach tail energy values are determined. By exciting the samples at 468 nm, the luminescence spectra were recorded and hence the radiative properties like luminescence intensity ratio (R), stimulated emission cross-section (σ) and branching ratio (β_R) values for the emission transition $^5D_0 \rightarrow {}^7F_J$ (J = 0, 1, 2, 3 and 4) of the Eu^{3+} ions were determined and reported. Furthermore, through 1931 CIE chromaticity diagram, emission spectra were characterized to explore the suitability of the prepared glasses for red laser and display device applications.

f) Surfaces, interfaces, and thin films

f0001

Phase Transition Studies in $Hf_{0.90}Y_{0.10}O_2$ Thin Films Deposited at Different Oxygen Partial Pressure Using PLD

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$Hf_{0.90}Y_{0.10}O_2$ epitaxial thin films on YSZ(100) substrate were prepared at different oxygen (O_2) partial pressures (100, 70, 30, and 10 sccm) by pulsed laser deposition. The effect of oxygen partial pressure on crystalline and local structure was investigated using X-ray diffraction (XRD), Fourier Transform Infrared (FTIR) spectroscopy and Soft X-ray Absorption Spectroscopy (SXAS). The surface composition of thin films was determined by X-ray photoelectron spectroscopy (XPS). The XRD and FTIR results confirm that the film phase changes with change in oxygen partial pressure. The structure of $Hf_{0.90}Y_{0.10}O_2$ films was orthorhombic ferroelectric at 100 sccm, and the structure changes to cubic for 70, 30, and 10 sccm oxygen partial pressure. SXAS O K-edge shows that the hybridization of O 2*p* orbital with metal 5*d* orbital changes with change in deposition pressure. The results enlighten a deeper understanding of crystalline and local structure of technologically important Y doped HfO_2 films used for dielectric and ferroelectric applications.

f0002

Reactive Electron Beam Deposited Yttria Stabilized Zirconia Thin Films under Varying Oxygen Flow Rate

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We report optical and surface morphological studies of Yttria stabilised Zirconia (YSZ) thin films deposited by reactive electron beam (EB) under varying O_2 flow rate. Optical constants and film thickness have been derived by analysing measured transmission spectra by employing suitable modelling/fitting. Estimated refractive index lies between 1.88 and 1.93 for O_2 pressure range, 0 to $1.8x10^{-4}$ mbar. Refractive index depicts an interesting trend which has been attributed to the varying film stoichiometry, ad-atom energy/film packing density. Extinction coefficient is of order of 10^{-4} for all the films and not affected substantially by O_2 flow rate. It indicates that there is no remarkable dissociation of YSZ films. Such stability is the attribute of adding Y_2O_3 to ZrO_2. Surface roughness measured by atomic force microscopy is ~ 1.5 nm for all the films and does not vary significantly for 0 to $1.8x10^{-4}$ mbar pressure range of O_2.

f0004

Existence of Twisted Magnetic Phase at Ni/Gd Interfaces at Room Temperature

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Rare-earth (RE)/transition metal (TM) ferromagnetic heterostructures with competing interfacial coupling and Zeeman energy provide a rich ground to study different phase states as a function of magnetic field and temperature. Interfacial properties and control in these RE/TM heterostructures provide an excellent opportunity to engineer the macroscopic magnetic response by tuning the interface dependent microscopic interactions between the layers. Using polarized neutron reflectivity (PNR), by adopting front-back surface reflectivity measurements at room temperature (RT), we have investigated interfacial magnetic structure of a Ni/Gd multilayer grown on Si substrate.

f0005

Evidence of the S-atoms sputtering in few-layer MoS_2 under 70 keV Ne-ion irradiation

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The generation of vacancies in molybdenum disulfide (MoS_2) under energetic ions has been studied in depth because of its potential use in electrical, gas sensing, and hydrogen evaluation reaction (HER) features. The crystallinity and stoichiometry of the synthesized few-layer MoS_2 have been characterized by Raman spectroscopy, EDX, and XRD, whereas the surface morphology has been investigated by scanning electron microscopy. In addition, in order to investigate the few-layer MoS_2 systems under the 70 keV Ne-ions fluence, we found that crystallinity decreases with ion irradiation fluence and completely amorphized above 3×10^{15} ions/cm^2.The EDX measurement reveals a deterioration in the stoichiometry (S/Mo atom concentration from 2.29 to 0.52) of the few-layer MoS_2 as the ion fluence increases. Which is directly relevant to modifying MoS_2's electrical, gas-sensing, and hydrogen evaluation reaction (HER) properties.

f0006

Pyro-Phototronic Effect in Ferroelectric Perovskite Thin-films and Photodetection

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We introduce $Cs_2PbI_2Cl_2$, an all-inorganic 2D Ruddlesden–Popper (RP) halide perovskite, as a ferroelectric material suitable for pyro-phototronic applications. Thin films of the all-inorganic perovskite are successfully fabricated and demonstrate ferroelectric properties. Leveraging these properties, we construct p-i-n heterojunctions by integrating the perovskite with carrier-transport layers. This design ensures a type-II band alignment at the two interfaces, enabling the material to exhibit both photovoltaic and pyroelectric behaviors when subjected to pulsed illumination. Unlike hybrid ferroelectrics, $Cs_2PbI_2Cl_2$ does not rely on an organic moiety with an electric dipole moment. Instead, a distortion in the bond lengths induces a twisting/tilting in the 2D-layer-forming octahedra, leading to the emergence of spontaneous electric polarization. The devices developed in this study harness the pyro-phototronic effect of the all-inorganic RP perovskite, serving as self-powered photodetectors without the need for any external bias.

f0008

Dynamic Wetting Behavior of Size-selected Ag-nanocluster Aggregated Films

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Abstract. In this report, we have studied the morphology and dynamic wetting behaviors of the films prepared by size-selected Ag-nanoclusters on pristine silicon surfaces. The films have been prepared in a state-of-the-art magnetron-based gas aggregation-type cluster deposition system. Beams of size-selected Ag-nanoclusters with an average diameter of ~ 4 nm have been utilized for the preparation of the films. The deposition time is kept fixed and the intensity of the beams is varied to developed films which contain surface coverage values from 24% to 41%. The topography of the films is investigated by atomic force microscopy (AFM) and field emission scanning electron microscopy (FESEM), respectively, and found that both the lateral and vertical sizes of the films along with the roughness evolved with the increase of the beam intensity. Dynamic contact angle measurements of the surfaces suggest that higher-density surfaces kept their hydrophobic behavior for a longer time in comparison to lower-density surfaces. X-ray photoelectron spectroscopy (XPS) analysis has been performed to study the compositional details of the films.

f0009

Role of Film Thickness in Optical, Structural and Electrical Characteristics of Sputtered Molybdenum Thin Films

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The molybdenum (Mo) thin films of different thickness were synthesized by radio frequency (RF) sputtering on a Quartz substrate in the presence of Argon gas. The optical, structural and electrical properties of these Mo thin films as a function of film thickness were investigated using Spectroscopic Ellipsometry (SE), Fourier Transform Infrared Spectroscopy (FTIR) and Keithley parametric analyzer respectively. The thickness of these films was found to be 150, 200, 250 and 300 nm measured by spectroscopic ellipsometry. Further, the SE reveals that the optical characteristics such as absorbance, refractive index and extinction coefficient increase with the increase in the thickness of the as-deposited Mo thin film. The FTIR Spectra confirm the formation of molybdenum thin films and the intensity of characteristic bands increases with an increase in the thickness of as-deposited Mo thin films. Moreover, the Keithley parametric analyzer reveals that the conductivity of the molybdenum films increases with increased thickness.

f0010

Unraveling the Ultrafast Charge Transfer Dynamics in $CsPbBr_3/Sb_2Se_3$ Nanocomposite

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Abstract: Integrating inorganic lead halide perovskites nanocrystals (NCs) with low-dimensional materials has emerged as a promising and effective approach to enhancing optical and electrical properties. This combination holds great potential for advancing various applications in optoelectronics and photonics. Here, we report the ultrafast charge transfer dynamics between semiconducting metal halide perovskite $CsPbBr_3$ NCs and Sb_2Se_3 nanowires (NWs) using steady-state (photoluminescence) PL and ultrafast transient absorption (TA) spectroscopies. The drastic reduction in PL intensity of pristine $CsPbBr_3$ NCs in the presence of the Sb_2Se_3 NWs is probably due to fast charge separation and transfer between them. This is further confirmed using ultrafast TA measurement that successfully describes photo-excited charge transfer from $CsPbBr_3$ to Sb_2Se_3 in a picosecond regime with a decay constant of 15 ± 1 ps. Our studies provide a new vision for perovskite-based solar cell and photodetector applications, presenting important insights and innovative approaches that may drive the next phase of progress in these technologies.

f0011

Effect Of Bi Addition On The Structural, Optical And Morphological Behaviour Of $In_{10}Se_{70}Te_{20-x}Bi_x$ Films For Optoelectronic Applications

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The bi doping in in-se-te alloy and its impact on surface morphology, structure, and optical behaviors have been investigated in the present paper. The transition from $in_{10}se_{70}te_{20}$ to $in_{10}se_{70}te_5bi_{15}$ composition modifies the structural phases as observed from xrd. Raman study infers the microstructural as well as phase formation in the films. The decrease in lattice strain and increase in crystallite size is associated with the surface morphology change as noticed from fesem. The composition variation in $in_{10}se_{70}te_{20-x}bi_x$ (x=0, 5, 10, 15 at %) films were checked from edx measurement. The uv-vis-nir data inferred the decrease in transmittance with bi% and also reduction in bandgap. The calculated static linear refractive index by different model at different bi% satisfies moss's relation. The transition from hydrophilic one to hydrophobic nature is observed with increase in Bi %. The obtained experimental results for the studied films may be used for various photonic and optoelectronic applications.

f0012

Self-diffusion and interface diffusion in crystalline and amorphous Ni/Ti multilayer: A molecular dynamics study

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Diffusion phenomena in crystalline and amorphous Ni/Ti binary multilayer systems have been simulated by Molecular dynamics (MD) technique in a wide temperature range of 473 K to 1600 K and compared with experimental results. Early formation of B2-phase (austenite) of NiTi alloy at the interface and new FCC & BCC Ti phases in Ti layer have been noticed for amorphous multilayer system which corroborates well with experimental results. By studying diffusion of Ni and Ti separately a very interesting difference has been noticed, self-diffusion being dominant in Ti and interface diffusion in Ni. In Arrhenius plot of diffusion coefficients two different activation energies have been found in temp regimes of 473-1000 K and 1200-1600 K. It indicates to two different mechanisms of diffusion in two different regimes of temperature.

f0013

An Analysis on Role of Dielectric Layers on Pentacene Based Phototransistors for Broadband Photodetection

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Organic photodetectors are extensively studied in the recent past due to their low cost in manufacturing, ease of processability, tunable wavelength detection and suitability for flexible/wearable devices. In the present work we have used the well-known organic semiconductor, pentacene, for the development of broadband photodetectors. The material was fabricated as a three terminal field effect transistor structure in bottom gate top contact (BGTC) fashion. In the case of a BGTC transistor based photodetectors, dielectric interface play a major role in the growth dynamics of the semiconductor layer. In order to elucidate that we have used different polymeric layers in different combinations such as PMMA/SiO_2, PS/SiO_2, HMDS/ SiO_2 and bare SiO_2. The fabricate devices are subjected to photo response analysis and the performance was analysed from the mobility, threshold voltage, responsivity and sensitivity. It has been found that, devices fabricated with HMDS dielectric layer gives the best performance with the mobility of 1 $cm^2V^{-1}s^{-1}$, the threshold of -9 V and showing the highest responsivity and sensitivity of about 258.49 AW^{-1} for 421 nm and 480.56 for 372 nm.

f0014

Surface Magnetic Study of Metal (Sr, Sc, and Cr) Doped M-type $BaFe_{12}O_{19}$ Hexaferrite Thin Films

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The hexaferrite thin films of compositions $BaFe_{12}O_{19}$, $Ba_{0.7}Sr_{0.3}Fe_{12}O_{19}$, and $BaFe_{11.5}T_{0.5}O_{19}$ (T: Sc and Cr) have been grown on Si substrate by Pulsed Laser Deposition (PLD) technique and stabilized in the magnetoplumbite (P_{63}/mmc) structure. Grazing Incidence X-Ray Diffraction (GIXRD) of the thin films at different in-plane rotations confirmed the growth of deposited thin films in preferred orientation of (203), (207), (1114), and (405) planes, where intensities of peaks varied with the in-plane rotation of thin films. The increase of the laser pulse energy enhances the surface roughness and particle size of the deposited thin films. The Magneto-Optical Kerr Effect (MOKE) measurements of the thin films showed the hysteresis loops of a typical ferro/ferrimagnetic material. The saturation magnetization of the thin film surface has not attained within the applied field range of ± 300 mT, indicating the hard ferromagnetic nature of the films. Un-doped and Sr doped at Ba-site thin films have shown a coercivity of ~ 112 mT, whereas Sc and Cr-doped at Fe-site thin films have shown a coercivity of ~ 146 mT. It has been noted that doping of Sr at the Ba-site does not affect much in the variation of coercivity, whereas doping of the Sc and Cr at the Fe-sites has enhanced the coercivity in the $BaFe_{12}O_{19}$ thin films.

f0015

Effects of the annealing conditions on the structural, morphological and mechanical properties of sputtered-deposited NiTi films

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In this study, NiTi films have been deposited on Si substrates by radio frequency (RF) and direct-current (DC) magnetron sputtering using elemental Ni and Ti as sputter targets. Samples were annealed at 600 °C in a vacuum and in an Ar medium to examine the impact of various annealing conditions on NiTi films. NiTi films were studied using X-ray diffraction, energy dispersive x-ray analysis, field emission scanning electron microscopy, atomic force microscopy, and nano-indentation techniques to determine their crystal structure, elemental composition, surface morphology, and mechanical properties. It was found that annealing NiTi films at 600 °C in various atmospheres can modify their structural, morphological, and mechanical properties. The grain size, surface roughness, and hardness of films that have been annealed in an Ar medium are enhanced compared to those of samples that have been annealed in a vacuum medium.

f0016

Investigation Of Optical And Magnetic Properties Of Thermally Evaporated Hematite Film On Alumina Substrate

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Hematite film has been grown on alumina (Al_2O_3) substrate by employing Thermal evaporation technique. GI-XRD confirmed the rhombohedral structure of the film. Multiple maxima and minima observed in the reflectance spectra correspond to multiple beam interference arising from air-film and film-substrate interfaces. Optical band gap in the range of 1.3 eV, absence of a sharp Morin transition around 260 K and observation of surface paramagnetism due to uncompensated spins are the highlights of the work.

f0017

Structural And Chemical State Analysis Of Cr_2O_3/Si/Cr Trilayer Thin Film

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Abstract. Cr_2O_3/Cr coatings of thickness ranging from 0.5-10 μm are commonly used to protect steel substrates from corrosion and enhance their mechanical strength. These coatings are also applied to safeguard organically coated packaging steel from corrosion-driven peeling of the organic coatings. However, in recent research, efforts are continuing to explore new materials and combinations that can further enhance corrosion resistance against harsh environmental conditions. In the present work, we investigated the effect of an intermediate silicon (Si) layer, inserted between the thin Cr_2O_3/Cr layers on a Si(100) substrate. By performing simultaneous X-ray reflectivity (XRR) and Grazing Incidence X-ray Fluorescence (GIXRF) measurements, we have examined the microstructural characteristics of the resulting $Cr2O_3$/Si/Cr trilayer thin film structure. Furthermore, X-ray Photoelectron Spectroscopy (XPS) measurements were also performed to evaluate changes in the oxidation states of chromium (Cr) resulting from the addition of Si layer. Our findings revealed that Si possesses a higher oxidation property than Cr, as it extracts oxygen from the Cr_2O_3 layer and forms its own native oxides. It is anticipated that such type of analysis might be beneficial in understanding the micro-mechanism at the interface medium to correlate their physical properties.

f0018

Evaluation of Mechanical and Electrical Responses of Highly Stretchable Free-standing Polymer Films

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Abstract. Nowadays, stretchable electronics are advancing rapidly in the diverse domains such as soft robotics, wearable electronics and bioelectronics. Here, conducting and stretchable films are produced by blending solvents (organic) like dimethyl sulfoxide (DMSO) and diethylene glycol (DEG) with the mixture of PEDOT:PSS and PVA. From Raman spectroscopy, it is observed that benzoid conformation of PEDOT transforms into quinoid after incorporation of DEG or DMSO with PEDOT:PSS/PVA. The morphology captured by atomic force microscope modifies from grains-like to stones- or rocks-like morphology in presence of solvents. Electrical responses for all the films are non-ohmic in nature following Pool-

Frenkel charge conduction phenomenon. With DMSO and DEG, current enhancement is observed drastically i.e., 18 and 5 times respectively at 5 V. After DMSO and DEG blending, the mechanical property of the films also modifies and become highly stretchable and flexible. Elongations at break (%) for PEDOT:PSS/PVA, PEDOT:PSS/PVA/DMSO and PEDOT:PSS/PVA/DEG films are 149, 449 and 550 % respectively.

f0019

Variation in radius of curvature of Self-Assembled Polystyrene Nanospheres and its effect on Magnetic Properties of CoO/Co Thin Films

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In the present study, the morphological and magnetic properties of CoO/Co (100 nm) nanocaps prepared by ion beam sputtering and electron beam evaporation technique are presented. These films were deposited on PS (Polystyrene) nanospheres (800 nm and 600 nm diameter) using self-assembled nanosphere lithography technique on Si (100) substrate. For a comparative study, these films were also deposited on flat Si substrate under same deposition conditions. Scanning electron microscopy (SEM) shows uniform distribution of nanospheres on Substrate. Magnetic properties were investigated at room temperature using vibrating scanning magnetometer (VSM) show enhancement in coercivity when the film is deposited on Polystyrene nanospheres of lower diameter.

f0020

In-situ Surface Preparation of h-BN Flakes for Device Applications

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Single crystal hexagonal boron nitride (h-BN) is a large band gap insulator, extensively used as a perfect insulating layer in van der Waals (vdW) systems and as a dielectric medium in the next generation of nanocapacitors. Growth morphology and the interfacial interplay between metal films on h-BN substrate have been studied significantly to form metal-insulator-metal (MIM) and metal-insulator-semiconductor (MIS) devices. For studying the intriguing growth mechanism of thin epitaxial metal or 2D films, in-situ surface preparation of the h-BN substrate is necessary. In this present study, we show low energy electron microscopy (LEEM) as a noble method to identify the presence of organic contaminants introduced during substrate transfer processing on h-BN flakes exfoliated on Si (100) substrate. Organic contaminants form fractal-like structures on the flake surface, which adds a large broad luminescence peak to the Raman spectrum of the h-BN flake. Here, we proposed a recipe for the in-situ removal of these organic contaminants and to form a completely clean h-BN surface, which involves vacuum annealing at 850 °C in LEEM. Further, epitaxial thin cobalt (Co) film was also grown on a clean h-BN/Si surface for studying the capacitance effect in MIS junction.

f0021

Stand-off Fabrication of Heat Resistive Superhydrophilic Silicon Using ND:YAG Laser

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We report nanosecond laser texturing of crystalline silicon with subsequent superhydrophilic and heat resistive properties. The samples are laser processed in ambient conditions in normal atmospheric pressure. Micro structures with micro/nano channels are evolved after processing which contributes to the wettability change of the silicon surface. The samples are characterized by XRD, FESEM, EDX and Raman spectroscopy. The contact angles are measured using an indigenously built contact angle goniometer. The samples show superhydrophilic nature after laser processing. Interestingly, the samples retain their inherent properties and super-wettability even after annealing at 200 °C for 8 hours. Such architectures could find applications in devices working in high temperature environments.

f0022

Silver Nanoparticle Thin Films Fabricated by DC Sputtering For Surface Enhanced Raman Scattering Applications

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This present work demonstrates a comprehensive study on the Silver (Ag) thin films fabricated by using D.C. sputtering method, followed by different characterizations using various techniques. The structural and optical properties of the Ag thin films were studied using X-ray diffraction (XRD) and Ultraviolet-Visible (UV-VIS) absorption spectroscopy. The morphology of the films and the size of the nanoparticles were examined with the images obtained from Field-Emission Scanning Electron Microscopy (FESEM) and Transmission Electron Microscopy (TEM), which provides valuable insights into the surface of the film and the internal nanostructures. The films, after confirmation of the successful fabrication and characterization, were used to identify the molecules of dye using the Surface-Enhanced Raman Spectroscopy (SERS) technique as the Ag films display

a good tunable surface plasmonic behavior and observed that these films have potential applications in enhancing Raman signals to higher values.

f0023

Study of Interfacial Interaction of Ceria Nanocuboids on Si and Quartz Substrates at High Temperature

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Ceria nanocuboids were synthesized using the hydrothermal method. The transmission electron microscopy (TEM) confirms the formation of ceria nanocuboids with a size ranging from 10 – 40 nm. Selected area electron diffraction (SAED) and X-ray Diffraction (XRD) confirm the FCC structure of ceria. The thermal stability of the as-prepared ceria is analyzed using thermogravimetry (TGA). The TGA shows that the ceria nanocuboids are thermally stable even at 1000 °C. The as-prepared CeO_2 is drop cast over Si and quartz substrates. The specimen was annealed at 1000 °C in a tubular furnace under N_2 atmosphere. The thermal stability of the thin film was investigated by analyzing XRD before and after annealing. Reflections corresponding to cerium silicate were found post-annealing.

f0024

Fabrication of High Temperature Resistant Superhydrophobic Coating on HVOF Thermal Sprayed Ni-Mo Surface

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Abstract
Industrial applications of metallic surfaces are impeded by major shortcomings due to persistent contact with water/moisture, such as damages owing to inadequate resistance to extreme temperature, corrosion-erosion under abrasive impacts, insufficient bond strength. Despite the existence of several traditional solutions, the application in challenging environments remains a significant issue. As a solution, in this work, we have fabricated a superhydrophobic coating via facile fabrication technique that can resist water adherence. Here, a high velocity oxygen fuel (HVOF) thermal spray coating technique was applied for spraying Ni-Mo alloy onto stainless steel (SS) surface, that has allowed to achieve the hierarchical framework of multi-scale roughness. Upon further surface modification with the low surface energy polymer, the superhydrophobic coating was achieved. The fabricated as-sprayed and modified coatings were studied for its surface properties and the effect of higher temperature. The obtained thermal stability test results revealed very good resistance of the coating towards extreme temperature, which was also observed via DSC and TGA analysis.

f0025

Bio-Inspired Soft Lithography for Fog Harvesting: A Sustainable Approach for Water Collection

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Abstract. This study shows the incredible skills of plants, such as their ability to regenerate and use bioenergy. The work uses soft lithography to transfer the Water Lily leaf surface pattern onto a polymer film. The surface morphology and structure of the polymer film are studied using optical microscopy. This leaf film was used to collect fog water and to create a Water Lily-Triboelectric Nanogenerator (WL-TENG) device. The main objectives of this research are to improve fog water collection efficiency, increase triboelectric nanogenerator efficiency, and reduce freshwater shortages in dry places. According to the experimental data, the Water Lily's roughness provides open-circuit voltage (V_{oc}) and short-circuit current (I_{sc}) peak values that can reach 338 V and 29.4 μA, respectively. In addition, the WL-TENG can power 15 commercial light-emitting diodes (LEDs) and a Lumex display.

f0027

Modeling of Growth of MoS_2 film in Two Zone Furnace CVD System

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In this paper, we present a modeling of growth of MoS_2 film in a two-zone furnace CVD system with sulfur and Molybdenum trioxide (MoO_3) as precursors. The calculations are based on Deal-Grove Model. The thermodynamic feasibility of the process for a range of synthesis temperature was also evaluated. The growth rate estimated from the model was found to be consistent with the reported growth in literatures.

f0029

SILAR Deposited Al-doped ZnO Films for TCO Applications

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Transparent conductive oxide (TCO) thin films such as indium doped tin oxide (ITO) and fluorine doped tin oxide (FTO) are widely used in electro-optical devices. In recent years, aluminum-doped zinc oxide (AZO) thin films have emerged as most studied materials for the efficient replacement of ITO/FTO due to its low-cost, non-toxic and abundant elements. In this work, we prepared AZO thin films on glass substrates using a low-cost and facile SILAR (successive ionic layer adsorption and reaction) method for different dipping/SILAR cycles. The structural, morphological and elemental studies are done using X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM) and energy dispersive X-ray analysis (EDAX), respectively. The deposited AZO thin film exhibit flower-like morphology and hexagonal polycrystalline wurtzite ZnO structure. The optical transmissions of the thin films are studied using UV-Visible spectroscopy. The transmittance of the AZO film decreases with increasing the dipping cycles/film thickness. The electrical conductivity of the AZO film is found higher for thicker film.

f0030

An electrochemical investigation of glucose oxidase at TiO_2/Si thin film modified electrode

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TiO_2 thin film was coated on (1 0 0) p-type silicon substrate by sol–gel process using Spin coating technique. The XRD pattern of the film shows the presence of most dominant silicon peak with (4 0 0) orientation along with peaks of mixed anatase and rutile phases of TiO_2. The crystallite size calculated using Debye-Scherrer's formula is 32 nm for the film post annealed at 550°C. The presence of Ti, O and Si elements is confirmed from EDAX measurements. TiO_2/Si as a working electrode, the electrochemical responses for glucose with different concentrations were studied in detail. The sensitivity of glucose is 2.40×10^{-4} A mM^{-1} cm^{-2}

f0031

RGO supported $MoTe_2$ nanohybrid for superior glucose sensing: Insights from theoretical simulations

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Abstract. The transition metal dichalcogenide $MoTe_2$ monolayer functionalized with the Pd atom has been recently reported as an excellent glucose (GL) sensor. The semiconducting $MoTe_2$ monolayer, when supported with a conducting 2D material like graphene, the GL sensing performance can be enhanced to a large extent. This work extensively investigates the GL sensing performance of the hybrid $MoTe_2$/rGO system using the First-principles Density Functional Theory (DFT) simulations. The adsorption energy of GL on the $MoTe_2$/rGO hybrid system is -1.4 eV. This increased adsorption energy is due to the change in conductivity of the overall system due to the stress induced in the system during the hybrid structure formation and expedited charge transfer, and strong orbital interactions between the GL and the $MoTe_2$/rGO system. The practicability of the $MoTe_2$/rGO system as a GL sensor is also evaluated. This research will give a solid theoretical foundation for the experimental fabrication of $MoTe_2$-based glucometers.

f0033

Influence Of Thickness On Composition, Morphology, And Electrical Transport In Cr-Substituted Mn-Ni-Sn Based Heusler Alloy Thin Films

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Abstract. In the present study, we have investigated the dependence of structural properties, surface morphology, and compositions of Cr-substituted Mn-Ni-Sn Heusler alloy films on thickness. UHV RF magnetron sputtering system was used to grow films, and their thickness varied from 8nm to 120nm by changing the deposition time of films on MgO (100) substrates. All the films were deposited at ~300°C and annealed at 800°C for 4 hrs. Film thickness (d) was estimated by XRR, and the typical growth rate was found to be ~4nm/min. All films have a cubic structure with a small admixture of a possible orthorhombic phase at room temperature. The crystallinity of the films improves with increasing thickness, and it could be due to the accommodation of the film–substrate interfacial strain resulting in the preferred oriented growth of the films. Films with d ~ 8nm have a continuous surface morphology with fine grain-like entities having average chemical composition $Mn_{1.4}Ni_{1.8}Cr_{0.002}Sn_{0.46}$. The d~20nm film shows continuous and smoother surface morphology, and its average composition is $Mn_{1.6}Ni_{1.58}Cr_{0.17}Sn_{0.63}$. The film with a thickness of d~120nm has a continuous surface with larger and densely packed grains. The average composition is $Mn_{1.51}Ni_{1.75}Cr_{0.21}Sn_{0.51}$ which is quite close to the target stoichiometry. This shows that as the film thickness increases, the overall chemical composition approaches that of the target, with a concomitant improvement in the surface morphology.

f0034

Local electronic structure of Sn white flower motifs on five-fold *i*-Al-Pd-Mn surface using scanning tunneling spectroscopy

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Abstract. Quasicrystals are aperiodic structures with long range ordering and their electronic stabilization is due to the existence of pseudogap at the Fermi level. In the present work, combined results of scanning tunneling microscopy/spectroscopy (STM/S) measurements establish the presence of a deeper pseudogap in the Sn white flower (SnWF) motifs compared to *i*-Al-Pd-Mn at room temperature.

f0035

Effect of TiCl4 Treatment on the Structural, Optical and Device Characteristics of Carbon-based HTL free Perovskite Solar Cells

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Perovskite solar cells (PSCs) have significant advantages over traditional silicon-based solar cells, as they can be easily and affordably manufactured on a large scale. However, the growth of halide perovskite-based materials is hindered by challenges such as long-term stability, non-uniform film formation, and recombination. These factors pose significant obstacles to the widespread adoption of these materials in various applications. Titanium tetrachloride (TiCl4) serves a critical function in perovskite solar cells (PSCs) as a passivation agent. It aids in achieving proper grain formation, leading to enhanced efficiency and improved stability in the cells. The impact of TiCl4 treatment on the TiO2/perovskite interface's crystallinity and device performance is evaluated and compared with devices that did not undergo TiCl4 treatment. The study examined the quality and crystalline properties of the MAPbI3 films by employing PXRD to understand the impact of TiCl4 treatment. The absorption range and optical behavior of the MAPbI3 films were analyzed using UV-Vis-NIR absorption. Notably, the comparison of device performance between TiCl4 treated and untreated devices revealed that the TiCl4 treated device demonstrated superior performance.

f0036

Abstract: We have used a novel sol-gel process to demonstrate the formation of Al doped Zinc Oxide (AZO) thin films and have used z-scan techniquefor studying the third-order nonlinear optical susceptibility of AZO thin films.For doped thin films, The hexagonal wurtzite structures are confirmed by X-ray diffraction (XRD) investigation. The crystallite size ranges from 15 to 30 nm. Images taken with a scanning electron microscope (SEM) demonstrate that the films have roughly homogeneous morphologies, consist of many flower-like aggregates with nanosized multipetals.The results of the current research show that adding Al to ZnO causes significant changes in the third-order nonlinear susceptibility. Additionally, we have demonstrated that the third harmonic generation is also affected by treatment with 370 fs laser pulses at 1030 nm.High second order nonlinear refractive index (n_2) with switching in nonlinear refractive index is observed for different doping concentrations.

f0037

Structural and Optical properties of oblique RF Magnetron sputtered zinc oxide thin film at different RF power

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Abstract. We report the fabrication of ZnO thin films deposited on glass substrates using radio frequency (RF) magnetron sputtering method. An oblique RF magnetron with substrate rotation arrangement was employed to grow ZnO films at various RF powers keeping all other parameters invariant. X-ray Diffraction (XRD), photoluminescence (PL) spectroscopy, and ultraviolet-visible spectroscopy, techniques have been used to examine the optical and structural features of thin films. The XRD spectra clearly show a strong diffraction peak (002) at about $2\theta = 34°$, that shows a single-crystalline thin film with a wurtzite crystal structure and preferred orientation. According to the Scherrer relation, the crystallite size was found to increase from 10.0 nm to 13.0 nm with the RF power. PL spectra show increased intensity with increase of RF sputtering power. With increasing RF strength, a slight change in the band gap energy was observed. The findings indicate that oblique RF magnetron sputtering offers a means to modifying the structural and optical characteristics of ZnO thin films, making it a promising technique for potential applications.

f0038

Design and Development of W/Si X-Ray Supermirror Using C Buffer Layer for Space Telescope Application

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Abstract. Pt/C and W/Si X-ray supermirrors are used in grazing incidence geometry Wolter-I focusing optics for high X-ray energy imaging in space telescope. Using Hitomi block method, 296-layer and 36-layer W/Si supermirrors have been designed which can reflect up to 69.5 KeV energy at 0.18° and 0.12° respectively. The interface property of supermirror with these high

number of layers is very critical. 3 Å thickness C buffer layers are added in the W/Si periodic multilayer and the variation of interfaces and bulk property of the layers with and without buffer layer have been characterized by specular and diffused X-ray reflectivity measurements. Finally, 36-layer W/Si supermirrors are deposited with and without C buffer layer, and characterized by high energy X-ray reflectivity measurement at 25 KeV using Indus-2 SRS.

f0039

Optical Characterization of PVDF type Thin Film using Different Geometric Phases with 4-Step Algorithm

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Laser based Optical Characterization has been done of a PVDF (Polyvinylidene Fluoride) type thin film using Interferometric Technique. We have used Mach-Zehnder Interferometer set up which is coupled with two polarizing beam splitters along with geometric phase shifter in reference arm. The other arm of that interferometer has been considered as object arm to place the transparent thin film i.e., PVDF. Here we have studied the Average Birefringence for all those three Thin Films, Birefringence non-uniformities of those thin films, non-uniform thickness of those thin films, Ratio between two refractive Indices and The Effects of stress on Birefringence. Four types of geometric phases with six sets of shifters have been introduced on the reference arm of the interferometer to characterize that thin film using phase shifting algorithm. The geometric Phase Shifters include Adiabatic geometric phase, Non-Cyclic Non-Adiabatic geometric phase, Cyclic Non-Adiabatic geometric phase, and Non-linear geometric phase. We have used only 4-Step algorithm for those phases on reference arm to get characteristics. We have also found the hologram of the thin film using digital holographic algorithm.

f0040

Comprehensive Investigation Of Preparation Conditions And Resistive switching In Bismuth Ferrite Thin-Films

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Decades of research have shown the enormous potential of bismuth ferrite to be applied in significant applications like photovoltaics, memory devices, gas sensors and photocatalysis. A major proponent of these applications is the parent distorted rhombohedral phase and the relative ease at which the phase can be changed to suit the application. However, it has always had the propensity to leakage current and unintended phase change. The present work explores the preparation of phase pure bismuth ferrite films and investigates their resistive switching properties. Probable reasoning for the lack of resistive switching with minor changes in the preparation conditions is investigated through surface morphology and X-ray photoelectron spectroscopy (XPS). The work also inspects the effect of doping with an aliovalent ion like calcium on resistive switching. Deeper insights into the structural chemical and the enhancement in resistive switching which occurred during the doping were probed through X-ray diffraction and XPS studies. The results provide direct evidence of how phase transition into the tetragonal phase can enhance ferroelectric and hence resistance switching properties of bismuth ferrite thin films.

f0041

Synthesis of Carbon Black-Prussian Blue Composite for H_2O_2 Sensing Application

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Abstract
Recently, there is an increasing demand in mimicking peroxidase activity using nanomaterials towards enzyme-free H_2O_2 sensing for detection of metabolites and biomarkers. Herein, prussian blue (PB) anchored carbon black (CB) was designed in which PB possess peroxidase-like activity while CB with large surface area and high conductivity efficiently enhanced catalytic performance. Electrochemical studies, XRD, UV-visible and FTIR spectroscopy confirmed the presence of PB on the CB. The composite exhibited good catalytic performances toward H_2O_2 detection with a sensitivity of 617 μA/mM/cm^2 and a low detection limit of 0.7 μM with a linear range of 0.01-10 mM. Furthermore, the proposed sensor can be used for metabolites and cancer biomarker detection.

f0042

Impact of ITO Surface Contamination on the Electronic Structure of DNTT/ITO Interface

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Electronic structures of DNTT thin films (of thickness from sub-monolayer to multilayer) on the clean and unclean ITO surface were investigated using photoelectron spectroscopy (XPS and UPS) to understand the role of the contamination of the transparent electrode on the hole injection barrier. The adventitious contamination layer was found to act as a spacer layer between the clean ITO substrate surface and DNTT molecular layer. As a consequence, hole injection barrier height, interface dipole, ionization potential, and partial charge transfer at the interface were modified significantly.

f0043

Effect of annealing on crystal structure of iron phthalocyanine thin films grown on Si (111) surface: 2D-GIXRD and HAXPES study

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Abstract: Metal Phthalocyanine based organic compounds e.g. Iron Phthalocyanine are extensively used in organic devices like OFET, organic solar cells, OLED etc. However, efficiency and performance of such devices depends upon the crystallinity of such molecules on substrate surface. Herein, we report on the effect of annealing on the crystal structure of Iron Phthalocyanine molecules grown in Si (111) substrate using physical vapour deposition. The crystal structure of the films was investigated using 2-dimensional glancing x-ray diffraction (2D-GIXRD) and quantification of thin films was carried out by hard x-ray photoelectron spectroscopy (HAXPES).

f0045

Plasmon Response Analysis of Evaporated Ultrathin Copper Island Films using β-distributed Oscillator Model

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Optical properties of ultrathin metal island films have been the subject of interest not only for fundamental research but also for the practical use in nanoplasmonic devices. In the present work, the optical properties of thermally evaporated ultrathin copper (Cu) island films are determined to investigate their thickness dispersive wideband plasmon response. The Cu films of thickness in the range of 4.5-23 nm are deposited on fused silica substrates using thermal evaporation. Surface morphology and ultraviolet to near infrared transmission of the island films have been measured using atomic force microscopy and spectrophotometer, respectively. Optical properties such as refractive index and extinction co-efficient of the films are determined by fitting the transmission spectra. The theoretical transmission spectrum is generated considering the Cu film as a two layer system employing an effective medium approximation for each layer and β-distributed oscillator model for complex dielectric function of Cu. The absorption co-efficient spectra show that the localized surface plasmon resonance becomes broad and undergoes red-shift with increasing thickness of the island films.

f0046

The assessment of fractal dimensions using Power Spectrum Density & its impact on the band gap and associated band-tails of SnS thin film

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Abstract: The effects of fractal dimensions on the optical properties of SnS thin films are investigated and discussed in detail. The topographical assessment of the SnS thin film is evaluated by an atomic force microscopy (AFM) image, which exhibits columnar granular grain structure. It is found from recorded AFM images that the surface roughness of the thin films increases as the thickness increases. The fractal dimensions of thin films are calculated through the power spectral density (PSD) formulation. The fractal dimensions decreased with increasing thickness, which led to increased surface roughness. The optical band estimation through the absorption spectrum fitting (ASF) method from the recorded transmission spectra reveals the decrease in the energy gap from 1.40 eV to 1.24 eV and the band tail from 250 meV to 293 meV with thicknesses of 100 nm and 250 nm. Such an assessment provides insight into choosing the right thickness-dependent optical band gap and band tail for solar cell applications.

f0047

Synthesis and Study of Cr_2N Thin Films by Reactive Sputtering

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Abstract. Nitrides of early transition metals are known to be synthesized in the energetically favorable mononitride (MN, M = Ti, V, Cr) composition. Unlike MN, their metal-rich bimetallic nitride phase (M2N) is not commonly investigated due to its higher formation enthalpy. In recent years, M2N compounds have been portrayed as interesting candidates for 2D MXene materials. In this work, we report a simple route for the synthesis of the Cr2N phase. We performed reactive nitrogen sputtering of a Cr target using a mixture of Ar and N2 gases and found that the CrN phases can be obtained when the partial N2 gas flow RN2 exceeds 20%. However, for lower values of RN2, a gradual transformation from bcc Cr to interstitial Cr(N) to a disordered Cr2N phase can be observed. Thermal annealing of the amorphous Cr2N at 973 K leads to the formation of a well-ordered Cr2N phase.

f0048

Solid State Welding Of Dissimilar Materials With High Pulsed Magnetic Field

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Abstract
Magnetic Pulse Welding (MPW) is a solid-state lap welding technique to join two dissimilar job pieces by high velocity impact. The joining in solid state welding is due to sudden plastic deformation at the job piece interface due to high velocity impact at certain impact angle caused by high magnetic fields. The quality of weld in MPW is directly influenced by the magnetic field and geometrical parameters such impact angle. Pulsed magnetic field is generated inside the tool coil by the discharge current of capacitor bank. It exerts inward pressure on the job piece, and accelerates it to impact at high velocity. 208 µF capacitor bank was charged up to 15 kV and discharges 210 kA in 6 turn disc coil with field shaper. 35 T magnetic field is produced inside the field shaper by the discharge current of 200 kA from capacitor bank. Solid state welding of Cu-Al and Cu-Ti are performed at these parameters. A good quality wavy pattern is seen at the weld interface of dissimilar material joining using MPW technique.

f0049

Effect of strain on the emergent interfacial magnetization in LSMO/LNO heterostructures

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The influence of strain and stacking sequence on interfacial ferromagnetism and exchange coupling in correlated oxide $LaNiO_3/La_{0.67}Sr_{0.33}MnO_3$(LNO/LSMO) heterostructures is investigated. LNO/LSMO heterostructures are grown on two different substrates (MgO and $SrTiO_3$ (STO)) yielded different strain for LNO and LSMO layers. Structural characterization through X-ray diffraction and reflectivity suggest growth of good quality strained layers in these heterostructures. Magnetometry measurements using SQUID show presence of exchange bias effect in the heterostructures grown on MgO substrates but not on the ones grown on STO substrates. This suggests that strain driven modification of interface exchange interactions. These interfacial modifications may result in charge transfer and orbital reconstruction and shall be studied using interface specific techniques such as polarized neutron reflectometry along with X-ray absorption spectroscopy.

f0054

Ion Irradiation Induced Structural and Morphological Modifications of Epitaxial $La_{0.25}Pr_{0.375}Ca_{0.375}MnO_3$ Thin Film

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We report on the modifications of structural and morphological properties of epitaxial $La_{0.25}Pr_{0.375}Ca_{0.375}MnO_3$ (LPCMO) thin film. LPCMO thin film of ~ 28 nm thickness were grown using pulsed laser deposition on the (110) $NdGaO_3$ (NGO) single crystal substrates. The deposited film was irradiated with 120 MeV Ag^{15+} ion beam varying fluence values of 1×10^{11}, 5×10^{11}, and 1×10^{12} ions/cm^2. X-ray diffraction study suggested highly oriented growth of the as-deposited film and the development of out-of-plane tensile strain in LPCMO film upon irradiation. The strain value was found to be higher for the higher ion fluence value. The morphology of the film was also found to be modified with the irradiation.

f0056

Optimized Third Order Nonlinear Optical Response in CuTPP Thin film by Virtue of Enhanced Electron Delocalization through Charge Transfer State and H-aggregation

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Nonlinear absorption (NLA) and nonlinear refraction (NLR) properties of Cu(II) 5, 10, 15, 20-Tetraphenyl-21H, 23H-Porphine (CuTPP) thin film at 532 nm is investigated by Z-scan technique with laser of pulse width, τ = 6 ns and 30 ps. Characteristic broad blue shifted soret absorption band with davydov splitting in UV-Visible spectrum and highlights the formation of H-aggregates. Emission peaks at 651 nm and 711 nm are attributed to de-excitation from $^2T_1$ and $^4T_1$ tripmultiplet states to ground state. At 30 ps pulse regime the NLA dynamics is influenced by saturation of tripmultiplet states and band filling effect, resulting in nonlinear saturation absorption phenomenon. Whereas, NLA at 6 ns pulse duration is influenced by excited state absorption of triplet states, resulting in reverse saturable absorption phenomenon. Closed aperture Z-scan depicts self-focusing

nonlinearity ($\Delta n>0$) at pico second regime. In nano second regime, CuTPP thin film depicts positive NLR at lower intensity and at higher intensity shows self-defocusing ($\Delta n<0$) NLR nature. Presence of charge transfer (CT) state in CuTPP molecule coupled with Van-der Waals interaction through π-stacking in thin film reciprocates exclusive nonlinear optical (NLO) properties.

f0057

Tuning Structures of Polymer Blended Organic Semiconducting Thin Films for Efficient Charge Transport

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Effect of blending insulating polymer to semiconducting polymer, on the quality of crystalline aggregates and their edge-on oriented ordering, particularly near the film-substrate interface, was investigated using optical absorption spectroscopy, X-ray reflectivity, and complementary atomic force microscopy techniques. The blended thin film shows better crystalline quality without altering the edge-on ordering near the film-substrate interface as compared to the pure thin film, which makes it better candidate for its use as an active layer in organic filed effect transistor devices.

f0059

Comparative Studies of Multiple PVDF type Thin Film Samples with Different Geometric Phases and Shift Algorithms

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A comparative analysis was conducted on Laser-based Optical Characterization techniques for various types of PVDF (Polyvinylidene Fluoride) thin film samples. The characterization process employed an Interferometric technique using a Mach-Zehnder Interferometer setup. The setup consisted of two polarizing beam splitters and a geometric phase shifter in the reference arm. The object arm of the interferometer accommodated the transparent PVDF thin film for analysis. The study focused on several parameters including the Average Birefringence of the thin films, non-uniformities in Birefringence, non-uniform thickness, the ratio between refractive indices, and the effects of stress on Birefringence. To characterize the thin film, four types of geometric phases were introduced in the reference arm along with six sets of shifters. Various phase shifting algorithms were employed, including 3-step, 4-step, 5-step, 6-step, 8-step, and 2n-step algorithms. Additionally, a least square fitting algorithm was utilized to extract the characteristics of these phases in the reference arm. Furthermore, the digital holographic algorithm was employed to generate holograms of the thin film. Through this comprehensive study, the aim was to investigate and compare the optical properties and behavior of different PVDF thin films using state-of-the-art interferometric techniques. The findings from this research contribute to a better understanding of PVDF thin films and their potential applications in various fields.

f0060

Enhanced Solar-blind Photodetection of Amorphous Gallium Oxide Thin Film using Nanopatterned Surface

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Ga_2O_3 is an ultra-wide band gap material with band gap > 4.4 eV, and hence is intrinsically solar-blind. Amorphous Ga_2O_3 based solar-blind photodetector have the advantage of simple and facile growth without the requirement of high temperature or lattice matching. However, their practical use is hindered because of the long response times. Herein, we report a simple and cost-effective method of nanopatterning its surface to enhance the device performance of amorphous gallium oxide thin film photodetector. Incident Ar^+ ion beam forms ripples on surface of gallium oxide thin film leading to anisotropic conduction channels being formed along with an increase in the surface defects. A reduction in the decay time of the devices even at self-bias, is achieved because the formed defects act as recombination centers, so much so that the fall time of the rippled devices reduces by more than 15 times. Thus, this work provides surface modification of Ga_2O_3 as a one-step, low cost method to increase the device performance of amorphous thin films, helping in the realization of next-generation optoelectronics.

f0061

Surface Functionalization of MoS_2 With ZnO For Highly Sensitive Room Temperature Nitrogen dioxide Gas Sensor

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Recently, 2D layered semiconducting material, MoS_2 has been widely researched for its gas sensing properties owing to its inherent high surface area, layer dependent physical and chemical properties and possible room temperature detection of gas analytes. However, pure MoS_2 based sensors often suffers from practical limitations due to their sensitivity and selectivity issues. In this study, ZnO nanoparticles were incorporated into MoS_2 sheets to modulate its electronic properties in order to enhance their gas sensing abilities. Optimized concentration of ZnO enhances the sensor response from 20 to 46 for 50 ppm NO_2 gas at room temperature with response and recovery time of 30 sec and 90 sec. respectively. Also the films are highly selective and stable towards NO_2 gas and shows the minimum detection limit of 200ppb. Formation of p-n heterojunction between MoS_2 and ZnO is mainly responsible for the superior sensing characteristics observed after functionalization of MoS_2.

f0063

Fabrication of Scintillator Thin Films via Controlled Deposition of CsI:Tl Microcrystals for Enhanced Radiation Detection

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Abstract The fabrication of CsI:Tl microcrystal thin films via the chemical route method presents a unique platform with significant potential in X-ray imaging and biomedical applications. The combination of efficient scintillation properties, facile fabrication over competitive techniques like RF sputtering and thermal evaporation technique, and adaptability to diverse substrates makes these thin films promising candidates for advancing imaging technologies and medical diagnostics.

f0064

Influence of Annealing Temperature on Optical Characteristics Based on Undoped and Mn-Doped Cs2AgInCl6 Nanocrystals for UV Photodetectors

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Abstract. Halide double perovskites have garnered significant attention in the realm of optoelectronic devices. The performance of these devices is intricately linked to the morphology of thin films, which in turn is influenced by the techniques employed for deposition and subsequent heat treatments. This work revolves around studying deposited undoped Cs2AgInCl6 and Mn-doped double perovskite nanocrystals (DP NCs) using the drop casting technique. Notably, an elevation in annealing temperature up to 300°C triggered a complete transformation of the perovskite phase into an alternative phase, as evidenced by X-ray diffraction (XRD) and steady-state photoluminescence measurements. The broad emission resulting from self-trapped excitons (STE) in undoped thin films was found to be heavily depends on the annealing temperature. To address potential optoelectronic device applications, a UV photodetector was fabricated and its photo response was assessed. Furthermore, UV-visible absorption spectroscopy, and device performance . This comprehensive approach provided insights into the bandgap change, crystallinity improvement and the photo response of UV photodetectors with undoped and Mn-doped $Cs_2AgInCl_6$ NCs.

f0065

Preparation and Characterization of Topological Insulator $(Bi, Sb)_2Te_3$(0001) Surface – an UHV STM Study

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Since last decade the surface of Topological Insulators (TI) have emerged as one of the most sensational states in quantum matter where surface host non-trivial electronic states originated from Dirac particles. $(Bi, Sb)_2Te_3$-based materials are one of the canonical examples of 3D topological insulators in which the Dirac point is located at the Fermi energy, essential prerequisite hosting elusive quantum anomalous Hall effect in magnetic doped TI. In order to probe the surface electronic structures using surface sensitive tools like scanning tunneling spectroscopy or photoemission experiment, typically samples are cleaved in vacuum to obtain fresh surface with well define atomic termination. In this work, we present the preparation of single crystalline $(Bi, Sb)_2Te_3$(0001) surface under ultra-high vacuum vacuo cleavage of bulk samples, followed by ion bombardment and annealing cycles. We established the optimized parameters for ion bombardment and *insitu* annealing process to achieve an atomically clean surface over general trend, which is cleaving the surface under vacuum. A detailed Atomic resolved STM and STS measurements shows interesting surface structures, various types defect geometry and influence of annealing on the general morphology the surface. Our procedure led to the favorable sample preparation in view of morphology and impurity density at the surface as compare to cleaved in vacuo.

f0067

Optical Properties of TiO_2 Composited Pr_6O_{11} Thin Films Deposited by Reactive Electron Beam Evaporation

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Abstract. In present work, composite thin films of TiO_2-Pr_6O_{11} have been deposited by reactive electron beam evaporation by varying oxygen flow rate. Optical constants and thickness of the films have been derived from suitable fitting of measured transmittance. Thickness of the films varies from 439 to 869 nm. Derived refractive index depicts an interesting trend of variation with O_2 pressure and it lies between 1.69 and 1.84. Its variation has been explained in the light of varying mutual concentration of different oxides of Pr and microstructural porosity. Extinction coefficient is lowest for film deposited without O_2 supply and is $6x10^{-4}$ at 1064 nm. It further increases with increased O_2 flow rate, but results in nearly similar values.

f0069

Synthesis and characterization of Ni-Ti thin films deposited by magnetron sputtering system

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NiTi thin films with thickness in nanometer regime were deposited by two sputtering modes. In first mode Ni-Ti thin films were deposited by sputtering from equiatomic NiTi target and in second mode Ni-Ti films were synthesized by co-sputtering from equiatomic NiTi alloy and Ti targets. It can be noted that films deposited by RF sputtering of NiTi alloy targets have higher oxygen contaminations, non-uniform distribution of alloying elements and are Ni-rich in composition. However, Ti-rich films were produced by co-sputtering from NiTi and Ti targets with minimal oxygen contaminations. It can be noted that with increase in sputter power, oxygen content in the film decreases which can be due to the formation of TiO_2 molecules during sputtering process. Annealing temperature of 650°C is required for Ti-rich films in order to convert amorphous structure to crystalline phase which shows Shape memory effect.

f0070

Interface Selective Study in Fe /^{57}Fe/ C_{60} bilayer; under X-ray Standing Wave Condition

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Abstract: Organic spintronics is one of the most advancing research fields for the last few decades. The interface of ferromagnetic metals and organic semiconductors plays a significant role in fabricating spin-valve devices. The magnetic properties of these interfaces play a vital role in the spin injection and extraction processes in organic spintronic devices. Present work employs the X-ray Standing wave (XSW) based grazing incidence X-ray diffraction (GIXRD) and grazing incidence nuclear resonance scattering (GINRS) in order to perform the structural and magnetic investigations. The diffusion of Fe clusters inside the C_{60} (fullerene) film with reduced hyperfine fields have been obtained in the diffused layers of ^{57}Fe at the interface. The possible cause of the reduction in hyperfine fields is due to the formation of small-sized Fe clusters exhibiting superparamagnetic behaviour.

f0071

Annealing Effects On Sputter Coated Ti Thin Films; Morphological And Raman Scattering Investigation

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A TiO_2 thin film is a wide band gap semiconductor material and it is used in photovoltaics, photo-catalysis and photo-sensors. In the present work, titanium thin films (thickness 50 nm)/Si samples are prepared by using DC magnetron sputtering system followed by annealing of Ti films at various temperatures in oxygen atmosphere. SEM analysis reveals that the grain size of TiO_2 increases with the annealing temperature. Raman scattering analysis show that the rutile TiO_2 phase is most prominent phase in the cases of annealing at 700 °C and 900 °C whereas signature of anatase TiO_2 phase is observed when annealed at 500 °C. The observations are consistent with literature.

f0073

Studies on Structural Properties of PVDF/MgO Nanocomposites

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Abstract: Polymer nanocomposites emerged as a new class of advanced materials due to their superior physical and chemical properties. A thin nanocomposite of Polyvinylidene fluoride (PVDF)/ Magnesium oxide (MgO) was prepared by the solution casting method. The crystalline structures of the nanocomposites were examined by the X-ray diffraction (XRD) method. The β-phase crystalline structure and surface morphology of the nanocomposite were studied using suitable characterization techniques. The MgO filler in PVDF plays a vital role in tailoring the surface morphology and thereby enhancing the β-phase formation in the nanocomposites.

f0074

Tuning the structural properties of $CoFe_2O_4$ thin film by varying thickness

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The thin film of Cobalt Ferrite was deposited on Si (1 0 0) substrate using the Pulsed Laser Deposition (PLD) technique with different thicknesses. The deposited film was characterized by Grazing incident X-ray Diffraction (GIXRD), X-ray reflectivity (XRR), and Raman Spectroscopy. GIXRD measurement reveals the formation of $CoFe_2O_4$ single phase and crystalline size increasing with thickness. X-ray reflectivity measurements suggest that the film thickness increases and roughness decreases with laser shots. As the thickness of the film increases, the oscillations within the XRR curve become denser. Furthermore, Raman spectroscopy measurement confirmed the formation of a single-phase cubic spinel structure.

f0075

Study of Functional Properties of ZrN Thin Films

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Refractory transition metal nitrides exhibit several functional properties. They are hard, metallic, and have extremely high melting points. In this work, we present our initial results on ZrN thin films grown using reactive nitrogen sputtering. A pure Zr sample was also prepared as a reference. Structural, superconducting and plasmonic properties of samples were studied. It was found that ZrN film with a lattice parameter close to its theoretical value can be obtained when deposited at a N2 partial flow ratio of 5%. The N concentration measured using Rutherford backscattering comes out to be about 47%. The electrical resistivity measurements confirmed superconducting nature of ZrN film with a TC of 3 K. The plasmonic response of ZrN film was found to be significantly superior than pure Zr. Obtained results are presented and discussed in this work.

f0076

Magnetic and Structural Asymmetry at The Interfaces of Ag/^{57}Fe/Ag Trilayer; Studies under X-Ray Standing Waves Condition

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Abstract: To understand and solve the existing ambiguities in the thin-film nanostructure, it is necessary to independently study interfaces (A-on-B and B-on-A) precisely in the same thin film structure to correlate them with existing properties such as TMR, DMI, PMA etc. [1]. Unfortunately, most of the techniques available either do not have sufficient depth resolution or do not probe true interfaces [2]. The availability of high-brilliance synchrotron radiation and its depth sensitivity under x-ray standing wave (XSW) has recently opened new avenues for applying the nuclear resonance scattering (NRS) method in the field of ultra-thin films [3]. High sensitivity and isotope selectivity of NRS is used to differentiate subtle changes in the magnetic structure at both the interfaces of Ag/Fe/Ag trilayer by placing a nuclear isotope ^{57}Fe. In addition, depth-resolved measurements under XSW conditions resolve the magnetic structure of both interfaces independently in the same trilayer. It is found that ^{57}Fe–on–Ag and Ag-on-^{57}Fe interfaces were not identical; 57Fe–on–Ag is more diffused, which was in good agreement with magnetic properties at both interfaces. However, it was in good agreement with interface roughness. With the thermal annealing, the Fe layer diffuses into the Ag layer, and after annealing at 375^{0}C, the trilayer becomes nonmagnetic. This is understood in terms of forming Fe nanoparticles in Ag matrix, which exhibited paramagnetic or super paramagnetic nature.

f0077

Enhanced Magnetic Anisotropy and Thermal Stability in Obliquely Deposited Co Film on the Nanopatterned Substrate

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Abstract: The deliberate manipulation of magnetic anisotropy through precise control of surface and interface morphology has sparked significant attention due to its promising application in spintronic and magnetic memory devices. The study

demonstrates enhanced thermal stabilization of uniaxial magnetic anisotropy (UMA) through controlled morphology on ripple-patterned SiO_2 substrate, combining oblique angle deposition (OAD) grown Co nanocolumns with ripple patterns. The present work reports the enhanced UMA after annealing these structures at moderate temperatures, contrary to the annealing effects reported previously. High-resolution synchrotron-based grazing-incidence small-angle and wide-angle X-ray Scattering unveils increased shadowing effects and column coalescence, resulting in stronger in-plane UMA. This work provides insights into morphological anisotropy, elucidating the interplay of shadowing effects, shape anisotropy, and dipolar interactions within magneto-elastically coupled ripple structures.

f0078

Temperature Dependent Thermoelectric Properties of Ag_2Se Thin Film in a Temperature Range From 150 K up to 430 K

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Bismuthe telluride (Bi_2Te_3) based alloys are the conventional thermoelectric materials for harvesting low temperature waste heat (<200°C). However, the toxicity of heavy element Bi, high cost of Te, low mechanical strength of Bi_2Te_3 based alloys have raised issues of concern. Recently mixed ion-electron conductor silver selenide (Ag_2Se) has received extensive attention due to its high figure of merit near room temperature accompanied with ecofriendly constituents. The Se vacancies that get generated during high temperature synthesis of Ag_2Se, act like donor impurities and make it intrinsically n-type. In this work we have synthesized thin film (thickness ~ 140 nm) of Ag_2Se on a Si test pattern. The temperature dependent thermocolectric properties including Seebeck coefficient, electrical conductivity, thermal conductivity, carrier concentration, mobility and dimensionless figure-of-merit of Ag_2Se thin film were measured in the temperature range of 150K-430K. The Ag_2Se film showed a highest figure-of-merit (ZT)~ 0.33 at 353 K.

f0080

Thickness Optimization of WO_3 Langmuir-Blodgett Films for Blocking Layer in Dye-Sensitized Solar Cell

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Abstract. Conventionally a thin (>50nm) spin coated/spray pyrolyzed TiO_2 film is employed as blocking layer (BL) in dye-sensitized solar cell (DSC) in order to reduce recombination. However, the thickness of BL has a significant effect on the blocking properties and therefore the DSC efficiency. In general, high blocking may be obtained for thick films but such high thickness results in reduced transparency and increased series resistance when employed in DSSC. In this work, we report thickness optimization of ultra-thin WO_3 BL prepared by Langmuir-Blodgett (LB) method. The optimized BLs show DSC efficiency of 6.5% and is attributable to excellent blocking and charge transport properties.

f0081

Cylindrical DC magnetron sputtering system for deposition of NEG based thin film for vacuum applications

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Abstract: DC Magnetron sputter system is a well-established technique for thin film deposition. In the present application, the thin film coating is required on the inner surface of cylindrical tube for vacuum pumping application. Traditional DC magnetron sputtering system is modified with twisted wire electrode and cylindrical deposition substrate for effective inner wall deposition of thin film. Wires of three different getter materials are twisted together for deposition in ternary alloy form in presence of electric field, magnetic field and Argon gas. The thin film gets activated at high temperature and adsorbs residual gasses thereby acting as vacuum pump at extreme high vacuum range. In the present article, the authors report the Cylindrical DC magnetron sputtering system which is used to deposit getter material on the inner surface of vacuum tube. In addition to the above, SEM, XPS characterization were performed to explore the surface morphology and elemental composition of the film.

f0082

Nitrogen (N^+) Ion Implanted Carbon Quantum Dots Derived From Mango Leaves (M-CQDs) Incorporated ZnO Hybrid Thin Films (ZnO/M-CQDs)

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Abstract. We have prepared the carbon quantum dots derived from Mango leaves (M-CQDs) incorporated ZnO (ZnO/M-CQDs) hybrid thin films. These films are then implanted with N^+ ion at low energy (25 keV) with high fluence of 5×10^{15} ions/cm². The High UV absorbance was observed for pristine ZnO when compared to the ZnO/M-CQDs and implanted films. N^+ ion implanted ZnO film exhibits highest optical band gap of 3.3 eV attributed to the compressive stress along out of plane. ZnO/M-CQDs hybrid film showed 2-fold enhancement in PL emission, ascribed to the charge transfer from incorporated M-CQDs to ZnO surface. XRD spectrum of ZnO exhibits hexagonal wurtzite structure and slight shift of (002) plane after N^+ ion implantation may be due to the effect of N^+ ions near film surface and formation of Zn-N bond.

g) Computational methods, and electronic structures

g0002

Understanding The Interplay of Eu/Sr and Tl in CsI matrix For Formation of Defect states through First Principal Calculation

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Abstract. Through first-principles calculations, we present our findings on the formation of deep level defects (DX-like centers) in Tl-doped CsI when co-doped with Eu or Sr. Our calculations indicate the formation of a defect complex (Tl^{-}_{Cs} + Eu^{+}_{Cs}/Sr^{+}_{Cs}) involving a cation-cation bond, rather than the isolated substitutional defect. This newly formed pair exhibits properties akin to a deep DX-like acceptor complex, which efficiently traps charge carriers responsible for the afterglow in CsI:Tl. Divalent doping has been demonstrated to remarkably improve afterglow suppression in CsI:Tl. These results shed light on the underlying mechanism of afterglow suppression.

g0004

Exploration of Electronic and Optical Properties of Chalcogenide Perovskite Materials AHfS3 (A = Ba, Sr) for Light-Emitting Semiconductors: First-Principles Study

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In this work, we have investigated the electronic and optical properties of $BaHfS_3$ and $SrHfS_3$ using the first-principles method based on the density functional theory (DFT) as implemented via WIEN2K program with the FP-LAPW method. The study reveals that both materials are forming perovskite structures with corner-sharing HfS_6 octahedra, and the optimized structure agrees with the available experimental data. Adopting the TB-mBJ functional for electronic structure calculations, we found that these materials have a wider direct band gap at the Γ center point along the high symmetry points in the Brillouin zone of 2.0 and 2.3 eV for $BaHfS_3$ and $SrHfS_3$, respectively. Further, optical studies reveal that both materials have a preferable absorption coefficient ($\alpha \sim 10^6$ cm^{-1}), the dielectric constant, and the refractive index for photovoltaic applications. They exhibit giant optical anisotropy as observed in many other quasi-one-dimensional chalcogenides. Direct band gap with the range of 2.0-2.5 eV and high absorption coefficient of the materials indicate their suitability in light-emitting semiconductor applications, which are critical components in designing optoelectronic devices such as light-emitting diodes, laser diodes, and solar cells.

g0005

Predicting Förster Critical Distance Using Machine Learning Techniques

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The efficiency of energy transfer between the donor (D) and acceptor (A) is a function of the Förster distance (R_0) in addition to other parameters, which can be determined experimentally at the cost of time and money. Can we have an intelligent approach that can estimate R_0 with a high degree of accuracy while costing minimal time and money without using a laboratory or experimental facility? For this purpose, we considered two well-established dyes, Rhodamine-6G (Rh-6G) and Rhodamine-B (Rh-B), as acceptors with other dyes as donors, and their related host (D/A)-guest (solvent/any solid) properties from the literature for predicting R_0 using the Machine Learning Regression (MLR) technique. For estimating R_0, we employed seven models, such as Linear Regression (LR), Decision tree regression (DTR), Random Forest Regression (RFR), AdaBoost regression (ABR), Extra Tree Regression (ETR), Gradient Boosting Regression (GBR), and XGBoost regression (XGBR). Out of seven, DTR outperformed other models in all four evaluation parameters: Mean Absolute Error (MAE), Mean Squared Error (MSE), Root Mean Squared Error (RMSE), and the coefficient of determination (R^2) values of 11.34, 130.52, 11.42, and 0.92, respectively. This 92% accuracy achieved with a small data set is the strength of the present study.

g0006

Crystal Structure, Hirshfeld Surface and Computational Nonlinear Optical Studies of Isonicotinohydrazide Derivative

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A new organic Nonlinear optical material ((E)-N'-(3,4,5-trimethoxybenzylidene) isonicotinohydrazide) monohydride (TBI) was synthesized by reflux method and the single crystals were grown by slow evaporation technique at ambient temperature using ethyl acetate as solvent. The crystal structure was determined using the single crystal X-ray diffraction technique. The crystal belongs to the monoclinic system with space group $P2_1/c$,cell parameters a =11.0217Å, b= 10.4992Å, c= 14.4003Å, V= 1657.19 $Å^3$, and Z=4. Optical transmittance of the grown crystal was investigated by using a UV–Vis–NIR spectrophotometer and obtained the optical parameters such as optical transmission bandwidth (270 nm to 800 nm), lower UV cut-off wavelength (365), and optical band gap (3.18 eV). Hirshfeld analysis was carried out to understand the packing pattern

and intermolecular interactions. Density functional theory (DFT) using the B3LYP/6-311G (d, p) basis set was utilized to analyze the frontier molecular orbital (FMO) of TBI. Besides, the static and dynamic nonlinear optical parameters (i.e., second and third-order hyperpolarizability) were estimated by employing the TDHF method with a basis 6-31G at different frequencies.

g0007

Nitrogen Reduction Reaction on TM-C_6N_6 : ML assisted DFT

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A series of transition-metal (TM) based single atom catalysts (SAC) embedded on carbon nitride (C_6N_6) have been chosen to explore the NRR activity. The promising metals have been primarily screened through density functional theory (DFT) by calculating their adsorption energies on C_6N_6 – energies for dinitrogen binding and the barriers at the rate determining step. Based on these criteria, amongst the 18 metal centers, Ta based C_6N_6 emerges as a good candidate for the reduction of nitrogen to NH_3. On the other hand, for the Machine Learning (ML) regression models, the covalent radius and the *d*-band center of the TM have been identified as the most correlated descriptors for predicting the adsorption energy of nitrogen on the active metal center. Besides, probabilistic modeling using the soft voting technique in the classification model shows, Ta based C_6N_6 dominates over the other catalysts which is in good agreement with DFT findings.

g0008

Impact of Graphene Layer Thickness on Switching Speed of the Vertical Organic Field Effect Transistor

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Vertical organic field effect transistors (VOFETs) are of paramount importance owing to their fast switching speed, low power consumption, and higher density on a chip and their potential to push the boundary of easy fabrication process based low cost flexible and biodegradable electronics. The incorporation of graphene in VOFET as a source electrode enhances the switching speed, when used in perforated manner. However, how the graphene layer thickness affects the switching speed of the organic field effect transistor in vertical geometry is still not clear. In this article, we simulate the graphene layer thickness dependence on the transfer characteristics of VOFET, wherein n-type organic semiconductor N, N′-dioctyl-3, 4, 9, 10-perylenedicarboximide (PTCDI-C8) is used as an active semiconductor material, perforated graphene as a source electrode, and aluminium (Al) as a drain electrode. The results suggest that the variation in the graphene layer thickness has the impact on the switching speed, where ON/OFF ratio changed from 106 to 102 from monolayer to 50 layers of graphene, respectively. The upsurge in the thickness increases the OFF current, while the ON current decreases and the transistor goes in saturation mode at even lower current density. The modification in graphene layer thickness changes the control of active channel and current modulation by the gate field, consequently the ON/OFF ratio value decreases. The findings will help in designing the perforated graphene source based VOFETs for improved switching speeds.

g0009

Electronic Structure Studies of $NdBaCo_2O_{5+\delta}$ (δ = 0,0.5)

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We have investigated oxygen deficient double perovskite cobaltites $NdBaCo_2O_{5+\delta}$ (δ = 0, 0.5), within the framework of density functional theory (DFT+U). These calculations were performed to understand the experimentally observed x-ray photoemission (xps) valance band spectra, thereby indicating the importance of onsite coulomb interaction in this class of compounds. We were able to reproduce experimentally observed valance band spectra using on-site Coulomb interaction term U for Nd *f* states (U_{Nd}) and Co *d* states (U_{Co})) with U_{Nd} / U_{Co} = 10.5 /5 eV and U_{Nd} / U_{Co} = 9.5 /5 eV for δ = 0 and 0.5 compound, respectively. To understand the cause for the metal to insulator transition (MIT) exhibited by these compounds detailed spectroscopic studies are vital.

g0010

Enhancing Vertical Organic Field Effect Transistor Performance: A Comparative Study between Floating and Non-Floating Source Contacts

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Vertical organic field effect transistors (VOFETs) offer high working frequency, current density, and low power consumption compared with the lateral organic field effect transistors counterpart. Simulation of the VOFET based on n-type N, N′-Dioctyl-3,4,9,10-perylenedlenedicarboximide (PTCDI-C8) using COMSOL Multiphysics software are carried out for improvement of device performance. VOFET performance is compared for floating and non-floating source contacts. Here floating source contact represents a contact which is not in direct contact with the gate dielectric. The simulations show that the non-floating contact has a higher current density than the floating contact due to less gate field penetration in the channel. The floating source contacts show improvement in VOFET performance by coating the top and side edge with insulator.

g0011

First Principles Study of Pressure Induced Phase Transition and Structural Properties of Li_2C_2

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Density functional theory calculations with van der Waals (vdW) force correction are performed to study the influence of static pressure on Li_2C_2. Pressure induced structural transition from *Immm* to *Pnma* phase has been studied. It is observed that calculations using PBE functional incorrectly predicts *Immm* phase to be thermodynamically unstable at ambient pressure, whereas, inclusion of vdW correction along with PBE functional established it to be thermodynamically stable. Further, it is demonstrated that inclusion of vdW effect reproduces experimental transition pressure of about 16 GPa while PBE-based calculation underestimates the same by about 21%. Moreover, compressibility of this compound is found to be different along three crystallographic directions.

g0012

Ab-initio Study Of $ZnMoO_4$ Under High Pressure

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We present a high-pressure study on -$ZnMoO_4$ using density functional theory (DFT) based calculations up to 50 GPa. Our investigation involves the full optimization of the wolframite and other four possible phases of $ZnMoO_4$ at different pressures. We also calculated their enthalpies and found that while -$ZnMoO_4$ is a metastable phase at ambient pressure, and becomes the most stable phase above 2.18 GPa. Further, we calculated its electronic band structure and density of states. These calculations show that -$ZnMoO_4$ is a semiconductor with an indirect band gap which decreases under pressure.

g0013

Electronic Structure of Antiferromagnetic $CuMnO_2$: A First Principle Study

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Geometrically frustrated $CuMnO_2$ has potential applications in photochemical cells, multiferroic devices etc. Electronic structure of anti-ferromagnetic $CuMnO_2$ was calculated using first principle methods under density functional theory (DFT). Electronic band structure, calculated under generalized gradient approximation (GGA) as well as GGA+U show indirect band gap of magnitude 0.51 eV (GGA) and 0.55 eV (GGA+U). Calculated total as well as partial density of states show that valance band is dominated by Cu-d and Mn-d orbitals while the conduction band is dominated by Mn-d orbitals. Three sharp peaks in the conduction band arise due to transition between crystal field split Mn-d orbitals.

g0014

Structural Stability and Electronic Properties of Armchair BN Nanoribbons With Selective Edge Functionalization

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Abstract. Tuning the electronic properties of nanomaterials is an active area of research. In this direction, present work reports the effect of selective edge functionalization on the structural and electronic properties of armchair BN nanoribbons (ABNNR). The H and Cl are considered as the functionalizing elements in various possibilities and the findings were compared with fully H-functionalized (pristine) ABNNR. It is predicted that partially functionalized geometries slightly improve their structural stability due to prominent edge reconstructions. Partially edge functionalization also exhibits a semiconductor to metallic transition irrespective of the ribbon width. The metallic structures (i.e. H-ABNNR, ABNNR-H and Cl-ABNNR) settled in the antiferromagnetic ground state except for H-ABNNR. An opening of a finite band gap was also observed with a magnitude of 2.12 eV and 0.78 eV in the magnetic state of ABNNR-H and Cl-ABNNR, respectively for width W=7. Furthermore, the magnetic stabilization energy is always greater than 350 meV which ensures their acceptance as magnetic materials for widespread applications.

g0015

Investigation of Structural, Electronic and Elasto-Mechanical Properties of Quaternary Heusler Alloy: GdTiYAl

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For the first time, we comment on the structural, electronic and mechanical properties of the Quaternary Heusler alloy GdTiYAl using an ab-initio approach. The Full potential linearized augmented plane wave (FP-LAPW) technique predicts the correct ground state parameters in generalized gradient approximation (GGA). Other elastic moduli and second order elastic constants were calculated. The calculated mechanical characteristics show that GdTiYAl is ductile and anisotropic.

g0016

Modeling and Simulation of Thermodynamic Properties of Metal and Alloys related to Nuclear Structural and Fuel Materials

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Thermodynamic property calculation of BCC iron with defects provides a large database of formation and binding energies of point-defects and their pairs for an extended set of alloying elements with Z=1 to 54. This presentation will discuss the computed solubility in comparison with those obtained from phase diagram database. This work reveal several fundamental trends in point- defect energies and size factors of solutes which will be useful for identifying alloying elements with desired diffusivity for optimizing coarsening kinetics and creep strength of steels. Stability of oxide particles in ODS steels will also be discussed on the basis of their formation energies in Fe. Our study on uranium with point-defects is an advancement compared to conventional DFT calculations because first-principles prediction of thermodynamic properties of high-temperature phases of solids is a challenge in materials physics and because thermodynamic properties of high-temperature BCC uranium with point-defects have been computed using FPMD simulations. Formation and binding energies of defects and their pairs besides bulk modulus and thermal expansion coefficients of uranium with these defects have been computed. Comparison of binding energies indicates that the nucleation and growth of fission gas bubbles is supported by a thermodynamic driving force over void formation through vacancies joining together.\

g0017

Exploration of Magneto-Electronic, Structural and Mechanical Properties of V_2MnGe Heusler alloy: A DFT Insight

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We have analyzed the structural, electro-magnetic and mechanical properties of Vanadium based Heusler alloy V_2MnGe. The alloy stabilizes in cubic phase with #216 space group. The alloy optimizes in ferromagnetic and non-magnetic phases showing stability in ferromagnetic phase. The total magnetic moment of this alloy is 3μB which is in accordance with Slater-Pauling rule. The electronic properties of the alloys show the metallic character in GGA and mBJ approximations. Elastic constants (like Pugh's ratio, Cauchy pressure etc.) display that the alloy is mechanically stable possessing ductile nature. The present study illustrates the consequence applications in research fields such as energy harvesting and thermoelectric technology.

g0018

An Ab-initio Study of Nickel Nano Clusters for Hazardous Gas Sensor Application

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In this study, the electronic structure and sensing properties of Nickel cluster Ni_n(n=2-6) using Density Functional Theory (DFT) are presented. The stabilities of the clusters are performed by calculating binding energies/formation energies, HOMO and LUMO gaps to know the cluster's affinity to adsorb and act as catalytic. Since Nickel Nano clusters involve chemical reactions with polluting gas molecules Hydrogen Cyanide (HCN) and Cyanogen chloride (CNCL) are adsorbed. We observed the binding energy for Ni_6 is -2.67 eV among all the clusters considered energetically favorable for the adsorption of gas molecules. Furthermore, the longer recovery time suggests that Ni_6 nanocluster could be considered as a promising candidate for removal material for HCN gas molecule from the environment, whereas shorter recovery time for CNCl gas molecule suggested that it can be used for detection purpose.

g0019

Image Based Machine Learning for Materials Science

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Materials research studies are dealing with a large number of images which can now be facilitated via image-based machine learning techniques. Raman spectroscopy is a powerful tool for the identification of chemical species in materials. This study proposes an artificial intelligence approach for rapid automatic detection of mineral samples from RRUFF database based on their Raman Spectra. The main part of the mineral detection system is the convolutional neural network, VGG16. Total 720 spectra from 24 minerals are used for learning process of neural networks. In this study, the performance of VGG16 over different network parameters is also considered

g0020

Evaluation of Simplified Density Functional B97-3C for the Simulation of Optoelectronic Properties of Biphenylyl/ Thiophene Derivative

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Organic optoelectronic materials present exciting prospects for the development of organic light emitting transistors and organic lasers. Realizing such devices requires materials with excellent mobility and high photoluminescence quantum yield. Theoretical methods provide valuable insights by modeling the optoelectronic properties of potential candidates, guiding experimental analysis. However, as the molecular complexity increases, computational costs and time escalate as well. To address this challenge, simplified methods like B97-3C have been developed and reported. This necessitate testing with various molecular systems and benchmarking against experimental and high-level theoretical results to establish them as standard techniques. In this study, we employ the B97-3C functional to simulate the structural and optoelectronic properties of the well-known 5,5″-bis(4-biphenylyl)-2,2′:5′,2″-terthiophene (BP3T) molecule and compare with previous data obtained using the B3LYP functional. The outcomes indicate that B97-3C satisfactorily reproduces the geometry and optical properties of BP3T. However, it significantly underestimates the LUMO values, resulting in a notable variation in the bandgap and electron drift mobilities.

g0021

Electronic and Magnetic Properties of Fe based MBenes

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Two-dimensional (2D) magnetic materials are promising candidates for future spintronic applications due to their lower thickness and low power consumption than the bulk materials (1). We explored Fe based 2D MBene by using first-principles density functional theory calculations within Quantum Espresso simulation package. A few Fe based MBenes with orthorhombic (O) and hexagonal (H) phases and various stoichiometric ratios (Fe:B) have been studied and their structural and magnetic ground states have been predicted, out of which O-Fe_2B_2, O-FeB, and H-FeB show antiferromagnetic ground state, while H-Fe_2B_2 shows ferromagnetic ground states. In the predicted magnetic ground state, properties of these Fe based MBenes can be further tuned for future antiferromagnetic-spintronic devices.

g0022

Electronic Structure of Antiferromagnetic Ce_3ZrSb_5 with Hypervalent Sb Chains

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We investigate the electronic structure of Ce_3ZrSb_5 (CZS), a material with a quasi-one-dimensional (1D) chain of Sb atoms as a potential candidate showing topologically non-trivial properties. The band structure calculations of CZS were carried out within the framework of density functional theory (DFT) using the full-potential linearized augmented plane-wave (FP-LAPW) method as implemented in the WIEN2k package. The DFT results reveal symmetry-protected band crossings in the vicinity of the Fermi level, E_F. Within the generalized gradient approximation (GGA), the density of states (DOS) near E_F exhibits a predominant Ce 4*f* and Sb 5*p* character. At finite Hubbard U, Ce 4*f* partial DOS (PDOS) near E_F exhibits significant change. With increasing U, the Ce 4*f* PDOS shifts away from E_F, revealing the underlying topological band crossings near the Fermi level. These results highlight the significance of 1D Sb-chains as a structural motif for identifying novel materials which may harbour complex magnetic and topological states.

g0023

Thermal effects on mc-Si ingot growth through directional solidification process with conventional and modified retorts: A numerical investigation

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Abstract. In this paper, the results of the ingots grown with the conventional retort and three modified retorts which are insulation inserted in bottom, centre, and top of the retort respectively are compared with each other. The heat dissipation was analysed 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 show 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.

g0024

X-ray Absorption Near Edge Structure Studies of Co_2MnAl and Ti_2MnAl

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We study here, structural, x-ray absorption near edge spectra (XANES) and electronic structure of X_2MnAl (X= Co, Ti) carried out at room temperature. Both the compounds crystallize in cubic structure with $Pm\bar{3}m$ spacegroup. The obtained lattice parameters are 5.76 Å and 6.20 Å for Co and Ti compounds, respectively. Our spectroscopic results show a direct link with the structural properties of the compounds.

g0025

Electronic Transitions in $BaPb_{1-x}Sr_xO_{3-z}$

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This study investigates metal to insulator transition (MIT) in $BaPb_{1-x}Sr_xO_{3-z}$ through density functional theory (DFT) calculations using local density approximation (LDA). The total density of states (TDOS) were calculated with varying levels of doping and oxygen deficiency. We found that two kinds of transitions occur in the material, (1) MIT upon doping of 25 percent of Sr in the Pb site, and (2) insulator to metal transition (IMT) by introducing oxygen deficiency in $BaPbO_3$. However, detailed experimental investigations are required to probe the above behaviours.

g0026

Study on Mechanical and Dynamical Stability of TiS_3 Under Pressure

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Due to numerous industrial applications, titanium trisulfide (TiS_3) has been the focus of extensive research like photo-voltaic and thermoelectric devices. Pressure may offer a way to enhance the physical or chemical properties of materials because of its well-known effects on inter atomic distances and crystal structures. Here, using density functional theory based first principles calculations we have studied mechanical and dynamical stability of TiS_3 at different pressures. Positive phonon frequencies as obtained from our phonon calculations confirm the dynamic stability of both ambient and high pressure phase of TiS_3. Further we found both the structures obey the Born stability criteria and hence are mechanically stable under pressure as evident from our calculated elastic constants.

g0027

Electronic, Optical and Mechanical Properties Of 2D Cu_2N Monolayer

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We implemented First-principles Density functional theory calculations to investigate the electronic, optical and mechanical properties of two-dimensional (2D) Cu_2N monolayer. The results shows that Cu_2N monolayer is metallic in nature at GGA+SOC level of theory. The tensile strength of Cu_2N monolayer is calculated to be 20.83 GPa. The optical absorbance spectra of Cu_2N shift from visible to ultra-violet (UV) region when the material transform from bulk to monolayer. We have also observed shifting of bands due to the impact of applied biaxial strain. The tunable properties of Cu_2N monolayer makes it potential candidate for nano electronic applications.

g0028

Special Features of Transmission Across an Emissive Complex Potential

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Tunnelling through a rectangular and delta barrier/ well with complex potential is explored. Expressions for transmission, reflection and absorption are obtained for both rectangular and deltapotential with emissive imaginary part. The variation of these quantities as a function of energy and strength of the complex part are studied and compared with the results for corresponding absorptive case. In contradistinction with the latter, in the case of emissive complex potential sharp peaks occur for transmission, reflection and emission for both of the potentials and they are investigated.

g0029

Enhanced Hydrogen Storage Capacity of Janus $GaAlS_2$ Monolayer by Metal (Li, Na, and K) Functionalization

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In the recent study, we have examined structural, electronic and hydrogen storage characteristics of Janus $GaAlS_2$ monolayer with the help of first principle computation. The semiconductor $GaAlS_2$ monolayer possess 2.87 eV band gap, indirect in nature. The adsorption energies of nH_2 (n=1, 2, 3, and 4) hydrogen molecules on $GaAlS_2$ sheet have been obtained. The functionalization of alkali metal (Li, Na, and K) on $GaAlS_2$ monolayer make the structure more appropriate for hydrogen storage. This is verified from suitable adsorption energies and desorption temperature of nH_2 molecules with Li@$GaAlS_2$, Na@$GaAlS_2$, and K@$GaAlS_2$ monolayers. These findings confirm the promising hydrogen storage ability of alkali metal (Li,

Na, and K) functionalized $GaAlS_2$ monolayer.

g0030

A First-principle Investigation on Optoelectronic Characteristics of $SnBr_2$/CuI van der Waals Heterostructure

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In present investigation, the van der Waals heterostructure (vdw HTS) is created by superimposing two distinct monolayers $SnBr_2$ and CuI using vdw force. The structural and optoelectronic characteristics of $SnBr_2$/CuI vdw HTS along with their pristine monolayers have been calculated by density functional approach. The energetic and thermal stability of $SnBr_2$/CuI vdw HTS is confirmed by the adhesion energy and AIMD calculation. The obtained electronic properties reveal that 2D $SnBr_2$/CuI vdw HTS has a direct 'Γ-Γ' type bandgap of 1.21 eV with HSE06 functional. It has type-II band alignment, which leads to an enhanced effective electron-hole pairs separation. Furthermore, the calculated absorption coefficient illustrates that $SnBr_2$/CuI vdw HTS exhibits an obvious red shift which leads to absorption in the visible region than the $SnBr_2$ monolayer. These comprehensive studies indicate that $SnBr_2$/CuI vdw HTS exhibits enhanced optoelectronics characteristics and has promising applications in UV-photodetector, nano-optoelectronic devices, and photovoltaic applications.

g0031

Elastic Properties of Bulk and Nano Gallium Nitride in The Presence of Universal Force Field

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Mechanical properties calculations give an insight of the materials strength, stress, strain, flexibility, elastic nature etc. Hexagonal GaN is a group III/V wide band gap semiconductor material known for its applications in various electronic devices, optical devices, spintronic etc. In this current research work, investigations on the mechanical properties of hexagonal GaN and armchair GaN (8,8) single walled nanotube (SWNT) are done using the universal force field by density functional theory approach. Universal force field used for computational parameters of interatomic molecular force field apply for all elements of the periodic tables. Using the Density functional theory, here various elastic parameters of hexagonal GaN and armchair GaN SWNT like young's modulus Y, bulk modulus B, compressibility K, Poisson's ratio σ, shear modulus G computed and analysed for further applications. Important structural and elastic behaviour of the material with 3D visualisation of the young's modulus, Poisson's ratio, linear compressibility and shear modulus is processed by the elastic stiffness constants Cij 6×6 matrix in an elastic tensor analysis (ELATE) software. Also the hardness, brittle or ductile, malleable, isotropic or anisotropic characters etc. of hexagonal GaN and armchair GaN (8,8) SWNT are studied.

g0032

Exploring the Radiation Resistance Behavior of bcc $Zr_{1-x}Nb_x$ ($0 \leq x \leq 1$) Alloy Solid Solutions: First–Principles Study

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Zr-based alloys are well-known as nuclear materials and have considerable importance, particularly in nuclear reactors. In the existing research works, the effect of irradiation on precipitate and microstructure stability in pure Zr with addition of 2.5% Nb have been reported. Hitherto, the impact of irradiation on intermetallic compounds of $Zr_{1-x}Nb_x$ alloy has not been studied in any detail. In this work, we have performed the ab-initio study of radiation resistance behavior of $Zr_{1-x}Nb_x$ alloys ($0 \leq x \leq 1$) considering sufficient high temperature where both Zr and Nb are completely solid solutions in bcc structure. We have calculated formation energy (ΔE) and formation enthalpy (ΔH) by creating defects (Zr or Nb vacancy at X = 0.5, Y = 0.5, Z = 0.5) in the structures. The result of formation energy with Nb concentration shows that Zr with 0% Nb has maximum ΔE, is hard to create defects, and has most stable structure. The solid solution is thermodynamically most stable at x = 0.5. Likewise, the same composition is found to be the most radiation resistant among the solid solution with $0 < x < 1$.

g0033

Critical Role of Exchange-Correlation Effects in Forming Dirac States in KZnBi

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Recent experiments identified KZnBi as a new three-dimensional Dirac semimetal with a pair of bulk Dirac states in contrast to the Z_2 trivial insulator reported earlier. To address this discrepancy, we have carried out the electronic structure and topological state analysis of KZnBi within the density functional theory framework. We find that various exchange-correlation functionals resolve a topological non-symmorphic insulator state with the glide-mirror-protected hourglass surface Dirac fermions. By carefully tuning the modified Becke-Jhonson (mBJ) potential parameters, we recover the correct orbital ordering and Dirac semimetal state of KZnBi. Our results demonstrate that KZnBi is a unique topological material where large electron correlations are crucial to realize the Dirac semimetal state.

g0034

Optoelectronic Characteristics of $ScYCT_2$ (T = Cl and Br) MXene Monolayers: Density Functional Approach

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The present research work represents the surface termination dependent electronic and optical properties of MXene ScYC monolayer. The $ScYCT_2$ (T = Cl and Br) monolayers have been theoretically studied. The surface of pristine metallic ScYC monolayer is modified by adding Cl and Br functional groups. The Perdew-Burke-Ernzerhof (PBE) of Generalized Gradient Approximation (GGA) and also hybrid exchange-correlation functional is incorporated for the band structure simulation. The results ensure the semiconducting behavior of $ScYCCl_2$ and $ScYCBr_2$ monolayers with indirect type bandgap of 1.93 eV and 1.63 eV, respectively. The Random Phase Approximation is employed for the simulation of optical characteristics, which suggests that the absorption starts in the infrared region and the utmost absorption found in the ultraviolet region. Hence, by surface modification, semiconductor $ScYCT_2$ monolayer has formed which has applications in optoelectronic devices such as UV detector, UV absorber, etc.

g0035

Designing Higher-Order Topological State in Square-Octagon Lattice with Staggered Magnetic Flux

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We investigate a square-octagon lattice with staggered magnetic fluxes for designing higher-order topological states in two-dimensional (2D) materials. We observe two types of topological states at half-filling, a topological Chern insulator with single-band inversion and a higher-order topological insulator (HOTI) with double-band inversions by systematic tuning of the hopping potentials at a particular staggered magnetic flux. The topological Chern insulator supports Chiral edge states, whereas HOTI forms in-gap topological corner states. These states stay preserved over an extended region of parameter space. Our study shows that square-octagon lattices provide a promising materials platform to realize topological states without time-reversal symmetry.

g0036

Tunable Intrinsic Superconductivity in $CsTi_3Bi_5$ with a Kagome Lattice

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ATi_3Bi_5 (A = K, Rb, and Cs) materials with Ti-based Kagome lattice exhibit various unconventional phases including non-trivial $\mathbb{Z}_2$ topology, electronic nematicity, and superconductivity but without any translational-symmetry breaking states. Here based on first-principles theoretical modeling and electron-phonon coupling calculations, we investigate the electronic structure and superconducting properties of $CsTi_3Bi_5$. The calculated band structure shows the coexistence of Dirac points, van Hove singularities (VHSs), and flat bands near the Fermi level that originate from the Ti-3*d* states. The calculated electron-phonon coupling strength at the Fermi level is 0.34 with a superconducting T_c of 0.13 K. We find that raising the Fermi level to the VHSs point enhances the electron-phonon coupling strength to 0.86 with an increased T_c to 5.66 K. Our study reveals that electron-phonon coupling strength and hence the superconducting T_c can be enhanced by tuning the electron filling in kagome lattice materials.

g0037

DFT Investigation on the Water Reduction Capacity of 001 Slab model of CdX (X= S, Se, Te) Structures

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Theoretical investigation were carried out on the water reduction capacity of slab models of Wurtzite CdS, CdSe and CdTe compounds, which is constructed in the 001 direction. For the systematic study, we are intertwining the relation between energetics of redox reactions and water reduction capacity of materials with the help of Density Functional Theory (DFT) calculations. We found polarization along the c axis of every CdX (X= S, Se, Te) unitcell structures due to the unsymmetrical tetrahedral structure, which leads to charge separation and better photocatalytic activity. Understanding this unique property of this wurtzite CdX structures, we constructed slab models along 001 direction and performed free energy analysis. Our findings reveal the inhibition of Cd-terminated surface for the water reduction reaction whereas all the chalcogenide surfaces provide highly favorable water reduction environment. Further, we also noticed the exciting water reduction capacity of S-terminated surface of CdS structures with a negative energy barrier of -1.28 eV, which is very less compared to all other chalcogenide surfaces.

g0038

Anisotropy in colossal piezoelectricity, giant Rashba effect and ultrahigh carrier mobility in Janus structures of quintuple Bi_2X_3 (X = S, Se) monolayers

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Due to their asymmetric structures, two-dimensional (2D) Janus materials have gained significant attention in research for their intriguing piezoelectric and spintronic properties. In the present work, Quintuple Bi_2X_3 (X = S, Se) monolayers (MLs)

have been modified to create stable Janus Bi_2X_2Y (X ≠Y= S, Se) MLs that display piezoelectricity in both the planes along with Rashba effect. The out-of-plane piezoelectric constant (d_{33}) is 41.18 (-173.14) pm/V, while the in-plane piezoelectric constant (d_{22}) is 5.23 (6.21) pm/V for Janus Bi_2S_2Se (Bi_2Se_2S) ML. Including spin-orbit coupling (SOC) in the Janus MLs results in anisotropic giant Rashba spin splitting (RSS) at the Γ point in the valence band, with RSS proportional to d_{33}. The Rashba constant along the Γ – K path, $\alpha_R^{\Gamma-K}$ is 3.30 (2.27) eVÅ, whereas along Γ – M, $\alpha_R^{\Gamma-M}$ is 3.58 (3.60) eVÅ for Janus Bi_2S_2Se (Bi_2Se_2S) ML. The MLs exhibit ultrahigh electron mobility (~ 5442 $cm^2V^{-1}s^{-1}$) and have electron to hole mobility ratio of more than 2 due to their tiny electron-effective masses. The flexibility of the MLs allows for a signification alteration in its properties, like band gap, piezoelectric coefficient, and Rashba constant, via mechanical strain. The coexistence of anisotropic colossal out-of-plane piezoelectricity, giant RSS, and ultrahigh carrier mobilities in Janus Bi_2S_2Se and Bi_2Se_2S MLs showcase their tremendous prospects in nanoelectronic, piezotronics, and spintronics devices.

g0039

A First Principles Study of 2D-2D CdS/MoS2 van der Waals Heterostructure

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Recently 2D heterostructures have attracted much attention in the field of photocatalytic water splitting. Here, we demonstrate 2D-2D van der Waals heterostructure CdS/MoS_2 with improved efficiency for the water splitting hydrogen production. We designed and explored the structural properties of CdS and MoS_2 monolayers and observed similar hexagonal atomic arrangement for both monolayers. By constructing the heterostructure, we aim to introduce interfacial dipoles inside the material, which will separate the charge carriers efficiently. For the analysis of electronic properties, band structure and density of states calculations were performed for the CdS/MoS_2 heterostructure and compared with those of isolated CdS and MoS_2 monolayers. The band gap of the heterostructure is indirect and obtained to be 1.19 eV. This Reduced band gap of the heterostructure indicates good visible light absorption, which is favorable for absorption.

g0040

Design of Novel Dual Janus Heterostructure PtSSe-SnSSe: A DFT Study

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Here, we are presenting designing of dual Janus hetereostructure for the solar assisted photocatalytic water splitting. The visible light active bandgap of the newly built heterostructure helps for the efficient solar light absorption for the charge separation. Moreover, the unique feature of built in electric field in the Janus structure as well as electric field created at the interface will be beneficial to improve the life time of charge carriers. This will reduce the charge recombination effectively and by reducing the charge recombination, there will be increase in the charge transfer to promote water redox reaction and hence the hydrogen production.

g0041

Stacking Independent Robust Thermoelectric Behavior In Magnetically Coupled $CrBr_3/NbSe_2/CrBr_3$ van der Waal Heterostructure

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The seamless integration of two-dimensional (2D) materials provides a potential platform to nurture numerous opportunities for advancing thermoelectric properties. Such 2D van der Waal heterostructures with enhanced charge transport mechanisms due to symmetry-breaking electronic configurations can offer a new pathway to realizing real-time thermopower devices. Herein, we study the electronic and thermoelectric properties of the $CrBr_3/NbSe_2/CrBr_3$ vdW heterostructure by employing density functional theory and constant relaxation time approximation (CRTA), respectively. The asymmetric bandstructure of designed heterostructure exhibits metallic ferromagnet behavior, which can be attributed to metallic d orbitals of Nb atoms. This exotic nature of electronic structure leads to enhanced thermoelectric characteristics with a higher Seebeck coefficient (S) and electrical conductivity of 414 μV K−1 and 1.28×10-20 Sm-1, respectively, in the vicinity of Fermi level at 250 K.

g0042

Non-Linear Optical Properties of Oxisulflower through Density Functional Theory Study

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In this work, using density functional theory (DFT) calculations we studied the structural, electronic and optical properties of superhalogen (BF_4) adsorbed oxisulflower systematically. The stability of all the adsorbed systems are predicted through binding energy. Adsorption of superhalogen on oxisulflower shows outstanding modification in their electronic as well as their structural and nonlinear optical properties. Superhalogen adsorbed oxisulflower has been seen to bring substantial changes in dipole moment, polarizability and first order hyperpolarizability of oxisulflower derivative. Overall, the theoretical investigation of non-linear optical properties on superhalogen adsorbed oxisulflower may be useful for future Non-Linear optical properties (NLO) materials.

g0043

***Ab initio* Investigation of Dielectric Functions of ZnS**

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Calculations based on the linear response time dependent density functional theory are used to investigate the complex dielectric function of ZnS. The ground state is obtained using first-principles Full-Potential Linearized Augmented Plane Wave method. After settling the crystal structure, band structure is calculated. The real and imaginary parts of the dielectric function are computed deploying adiabatic local density approximation of the linear response theory. Additionally, the random phase approximation is also considered. We have analyzed the effect of local field on peak intensity of the imaginary part of complex dielectric function. The interband transitions responsible for the structures in the spectra are specified.

g0044

Investigating Topological Quantum Phase Transitions in the Halide Perovskite Family via. Strain Engineering

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In this work, we have conducted first-principle electronic structure calculations to investigate the influence of strain and inversion symmetry breaking (ISB) field on the band topology of halide perovskites. Our findings reveal that the presence of the ISB field induces a discontinuous phase transition from a normal to a topological insulator state. In the absence of ISB, the system undergoes a gapless state before acquiring a non-trivial band gap with inverted characteristics. However, the introduction of the ISB field disrupts the stabilization of the gapless state, leading to a discontinuity in the band gap with the strain, resulting in a first-order topological phase transition.

g0045

Theoretical Explorations of Moiré Patterns in Twisted Bilayer $MoSi_2N_4$

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Moiré patterns have been recognized for their ability to confine electronic states within bilayers of graphene and transition metal dichalcogenides, thereby extending the concept of magic angles observed in the realm of semiconductors. Here, we use first-principles calculations to develop the idea of Moiré patterns in twisted bilayer $MoSi_2N_4$, a prototypical septuple-atomic-layer material. We show that Moiré superlattice's structural reconstruction occurs under geometric relaxation. Furthermore, band width shows quadratic dependence on the twist angle. Additionally, flat bands appear for the twist angles smaller than 3.48°. Moreover, the valence band edge states are real space localized on the specific high-symmetry stackings depending on the twist angle. Therefore, our calculations reveal that twisted bilayer $MoSi_2N_4$ holds great potential in the field of twistronics.

g0046

Electron Energy Loss Rate in Silicene due to Inplane Acoustic Phonons

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The electron-phonon interaction at low temperatures is essential in determining the novel thermoelectric properties of low-dimensional materials. Motivated by this, we numerically and analytically investigated the electron excitation and subsequent electron energy loss rate in Silicene, a two dimensional allotrope of silicon, with honeycomb two dimensional structure similar to Graphene. The scattering through in-plane acoustic phonon modes interacting via the deformation-potential coupling constant in silicene as a function of electrons temperature and electron density in the Bloch-Gruneisen regime and the related power dependencies have been determined . The results suggest that the magnitude of energy loss rate increases with temperature for
the different values of carrier density but shows non-monotonic behavior as the magnitude value first increases and attains a maximum and then decreases further throughout the complete Bloch-Gruneisen regime. This study is meaningful in estimating the electrical and thermal properties of silicene and in the fabrication of devices based on it.

g0047

Electronic Structure Studies of $NdBaCo_2O_{5+\delta}$ (δ = 0,0.5)

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We have investigated oxygen deficient double perovskite cobaltites $NdBaCo_2O_{5+\delta}$ (δ = 0, 0.5), within the framework of density functional theory (DFT). These calculations were performed to understand the experimentally observed x-ray photoemission (xps) valance band spectra. We were not able to reproduce experimentally observed valance band spectra with our DFT calculations for δ = 0 and 0.5 compounds, which indicates the importance of onsite coulomb interaction (U) in this class of compounds. To understand the electronic structure and cause of metal to insulator transition for these compounds, DFT+U calculations combined with detailed spectroscopic studies will be vital.

g0048

Density Functional Investigation on the Structure, Electronic and Optical Properties of $(CaO)_{6n}$ (n=1-8) Nanoclusters

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This paper presents a comprehensive analysis of the structural, electrical, and optical characteristics of the $(CaO)_6$ cluster unit within the $(CaO)_{6n}$ series, where n ranges from 1 to 8. The examination is conducted using a systematic density functional approach. The electronic characteristics of $(CaO)_{6n}$ nanoclusters are examined in relation to the HOMO-LUMO gap (HLG), ionization potential (IP), electron affinity (EA), chemical hardness (η), and electrophilicity index (ω). These properties exhibit a zigzag pattern as the size of the $(CaO)_{6n}$ clusters rises. The clusters were found to exhibit a significant increase in electronic energy (ΔE), leading to the identification of a very stable nanocluster referred to as a 'magic' nanocluster, namely $(CaO)_{36}$. The investigation of frontier orbitals in the $(CaO)_{36}$ nanocluster system reveals a propensity for facile electron transfer. The optical absorption spectra indicate that the $(CaO)_{36}$ nanocluster exhibits distinct quantum dot properties, making it visually detectable and holding promising potential for future applications.

g0049

Statistical Uncertainities in Molecular Dynamics Simulations of Material Response to High Strain Rates and Collision Cascade Simulations

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The role of statistical uncertainities in molecular dynamics (MD) simulations in two widely addressed problems in computational materials science, viz., (i) stress response to strain to study the Hall-Petch effect and (ii) collision cascades to study irradiation induced damage in materials, are addressed in this document. In the former we show the uncertainity in material response arising from both, number of grains used in the simulations (Fig.1-a) and the configurations of the grains taking Cu with a mean grain size of 10 nm as an example. In the latter we discuss the uncertainities arising from both, the direction of launch of the primary knock-on atom and that arising from the interatomic potential used, taking collision cascades in W as an example (Fig.1-b).

g0050

A Comparative Study On Structural, Electronic and Optical Properties Of Wurtzite ZnS and ZnAuS : A First Principle Calculation

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The structural, electronic and optical properties have been investigated of pristine and Au doped wurtzite ZnS by DFT based first principle calculation using Generalized Gradient Approximation (GGA) implemented in SIESTA code. The band and electronic structure study of pristine and Au doped ZnS were carried out which shows a narrowing and upward shift of valance band maxima (VBM) of doped ZnAuS than ZnS because of the introduction of impurity acceptor level, which overlaps with Fermi energy level due to hybridization of Au-5d and S-3p atomic orbitals, hence there is increase in p-type charge carriers. The optical property calculations like Absorption Coefficient, Reflectance, Refractive Index and Dielectric analysis shows optical isotropy in all directions. The results shows outstanding variation of optical properties with respect to change in wavelength in IR, Visible and UV region of spectrum, making it a potential candidate for various opticoelectronic based applications.

g0052

First-Principles Studies on Fe-Zr Alloys as Host Matrices for Nuclear Waste

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Energetics of s-, p- and d-block FMs, viz., Rb, Sr, In, Sn, Sb, Te, Cs, Ba, Y, Nb, Mo, Tc, Ru, Rh, Pd, Ag in the c-Fe_2Zr, t-$FeZr_2$ and o-$FeZr_3$ intermetallic phases were studied using density functional theory simulations. It has been found that s-block FMs are less weakly bounded to the intermetallics than the p− and d−block FMs. The solution energies of p− and d−block fission atoms are either slightly positive or negative. The high solution energies of s-block FMs suggest that these FMs are highly insoluble in the Fe-Zr intermetallics. The solution energy hierarchy of the FMs follow the trend as Cs>Rb>Ba>Sr>Ag>Cd >Y>Mo>Nb>In>Te>Sn>Tc>Sb>Pd>Ru>Rh. We also report the site preferences of these FMs in Fe-Zr intermetallics based on their solution energies.

g0053

Theoretical Study of Oxygen Functionalized group-III ternary chalcogenide monolayer compounds $MNTe_2$ (M, N = In, Ga, Al)

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The theoretical study of the 2D Oxygen Functionalized group-III ternary chalcogenide monolayer compounds **(**G3TCM**)** $MNTe_2$ (M, N = In, Ga, Al) have been done using density functional theory. $MNTe_2$ monolayer has a hexagonal structure. $MNTe_2$ monolayer is functionalized with an Oxygen atom using van der Waals corrections. The functionalized monolayers have shown the semiconductor behaviour. The $MInTe_2$ is thermally stable. Electron Localization Function (ELF) is also calculated for $MNTe_2O$. The calculated optical absorption coefficient has shown absorption in the infra-red, visible and ultraviolet regions which shows the potential application in optoelectronic devices and its applications.

g0054
Structural And Electronic Properties Of $TmAl_3$ Intermetallic Compound: A DFT Study
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The structural and electronic properties of isostructural and isoelectronic magnetic $TmAl_3$ intermetallic compound, which crystallize in $AuCu_3$-type structure, are studied using first principles density functional theory based on full potential linearized augmented plane wave (FP-LAPW) method. The calculations are carried out within LSDA for the exchange correlation potential. Our calculated ground state properties such as lattice constant (a_0), bulk modulus (B) and its pressure derivative (B') are in good agreement with the available experimental and other theoretical results. The computed electronic band structure and DOS reveal that the compound is metallic in nature.

g0055
Formation, Mass Spectrometric Stability & Charge Transfer Interactions in Subnanometer Sized Oxygen Deficient Lanthanum Metal Clusters
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Subnanometer sized lanthanum oxide clusters were produced in a recently built metal cluster beam setup by gas phase chemical reaction of laser vaporized La metal plasma with oxygen followed by supersonic cooling in a helium gas expansion. Time of Flight Mass Spectrometry were used to investigate the mass spectrometric stability of oxygen deficient neutral La_mO_n (m = 1–13, n = 1–6) clusters. All sizes could be produced in good abundance without the magic behavior of any cluster size. Density function theory has been used to determine the geometric structure, ionization energy, and charge transfer interaction of the neutral and cation La_2O_n (n = 1-4) clusters. Mulliken and Hirshfeld charge analysis indicate that the chemical bonding between the La and O is ionic while the bonding between the two La atoms is covalent. Threshold photoionization occurs from highest occupied molecular orbitals (HOMOs) which are predominantly metal based d orbitals.

g0056
First Principles Investigation for Electronic and Elastic Properties of Zinc Antimonide
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Density of states and energy bands have been derived by using linear combination of atomic orbitals (LCAO) method within the density functional theory (DFT). We have incorporated a hybridized approach for exchange energy, namely Predew-Burke-Ernzerhof (PBE) and Hartee-Fock (HF) exchange energies, known as PBE0 scheme. The mechanical properties have also been deduced to confirm the mechanical stability of ZnSb. The elastic properties obtained are in good agreement with previously reported theoretical and experimental results. ZnSb exhibits promising applications because of its low cost and low thermal conductivity and as a semiconductor in photo-optic devices.

g0057
Effect of Charge Carrier Mobility in Channel vs. Source-Drain Region on Vertical Organic Field-Effect Transistor Performance
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Lateral organic field-effect transistors (OFETs), due to lithographic limitations, have channel lengths ranging in micro-meters. Vertical organic field-effect transistors (VOFETs) have a channel perpendicular to the gate dielectric which means source and drain electrodes are vertically stacked. The vertical stacking of source and drain electrodes and due to the proximity leads to high off-state current density. There have been multiple efforts to reduce the off-state current and increase the on-state current. The presented simulation work explores the effect of different charge carrier mobility in source-drain region vs. channel region. In general, the charge carrier mobility in organic semiconductors increases with an increase in charge carrier concentration. The simulation results show that by enhancing the charge carrier mobility of the channel region by 10^3 orders, the best device performance can be achieved.

g0058

Study of Impurity effect on strongly correlated Heavy fermion system and to explore influence of the interaction of phonon with 'f' and 'd' electrons on resistivity a small 'q' and finite 'T' analysis

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Abstract: Here we tried to explore the effect of impurity and interaction of phonon with f and d electron on the electrical resistivity in some intermetallic strongly correlated heavy fermion (HF) systems. The temperature dependence of resistivity for finite wave vector (q) and for finite temperature (T) has been analyzed in the presence of the electron-phonon interaction by using Periodic Anderson Model (PAM). The Zubarev type Green function technique with double time and temperature dependence has been taken as the resistivity is related to the imaginary part of the electron self -energy. In this paper we studied the influence of various system parameters such as electron-phonon coupling strength g, location of zero energy level E_0, position of the f level d on resistivity has been examined. The result found has good agreement with the experimental remark.

g0059

A Theoretical Study On Structural, Electronic, and Mechanical Properties of $ZrBeO_3$ Perovskite

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The materials with a high potential for use in solar cells have been regarded as lead halide perovskites. However, the instability and toxicity of lead problems continue to be significant barriers to their widespread use. The present paper investigates structural, electronic, and mechanical properties of lead-free $ZrBeO_3$ perovskite via Wien2k software based on the full potential linearized augmented plane wave method using density functional theory (DFT), a first-principles method. The band structure and density of states are determined for the electronic characteristics, indicating the compound has a bandgap of 0.85 eV. Ground state properties like bulk modulus, a derivative of bulk modulus, ground state energy, and volume have been calculated from Birch-Murnaghan fitted curve. Mechanical properties reveal that the compound is brittle in nature. There is ionic bonding between Zr-O, Be-O, and Zr-Be pairs reflected by the electron density plot. It could find applications in the area of the solar energy field.

g0060

Kerr Effect of Titanium Dioxide: Microscopic Insights

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The microscopic mechanism of nonlinear refraction of titanium dioxide (TiO_2) and its dispersion is investigated from ab-initio simulations based on time-dependent density functional theory (TDDFT). This work demonstrates the application of TDDFT calculations to identify the mechanism of nonlinear optical interactions which will potentially enable future nonlinear photonic technologies. In this regard, the nonlinear refractive index (n_2) of TiO_2 at 800 nm and 400 nm are extracted from the intensity dependence of phase shift of photo-induced current and our results are in reasonable agreement with the existing literature. We observe that the n_2 is positive for off-resonant 800 nm while it is large but negative for resonant interactions at 400 nm. The large negative n_2 at 400 nm is due to the excited free carriers while the positive n_2 at 800 nm is originating from nonlinear refraction due to bound electrons.

g0061

First Principles Study of the Adsorption of Toxic Heavy Metals from Aqueous Solution on the Surface of Carbon Fullerene (C_{20}) for Environmental Remediation

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Heavy metals are generally referred as high atomic weight metallic chemical elements that could pose risks to the environment and living organisms. Some of the metals that pose health risks to humans are necessary at trace levels but are toxic at higher levels (Iron) while others are toxic with no known benefits (Nickel, Lead). C_{20} nanocage (C_{20}) called as endohedral fullerene has attracted the scientific community towards Bio-sensors, Drug delivery, Cancer therapy and Environmental remediation applications. The present work deals with the investigation on the sensing ability of C_{20} cage towards Toxic Heavy Metals (THMs) using Density Functional Theory (DFT) implemented in Gaussian 16 software package. where the THMs ($FeCl_3$, $NiCl_2$ and $PbCl_2$) are act as adsorbate and C_{20} cage act as adsorbent. The geometries of THMs, C_{20} cage and their complexes

(C_{20}+THMs) were fully optimized at B3LYP/LANL2DZ level of theory. From the adsorption energy, $FeCl_3$ [-48.19 kcal/mol] gets adsorbed well by C_{20} than $NiCl_2$ and $PbCl_2$. The negative sign indicates that there is a strong interaction between THMs and the C_{20} cage. Moreover, the THMs adsorbed C_{20} cage exhibit excellent optical behaviour compared to pristine C_{20} cage and THMs respectively.

g0062

Molecular Dynamics Study of Successive Primary Knock-on Atom Simulations in Zirconium

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Molecular Dynamics (MD) simulations of collision cascades with successive primary knock-on atom (PKA) simulations have been carried out in Zirconium. The simulations have been performed for PKA energy of 10 keV & 20 keV using the open source code Large Atomic/Molecular Massively Parallel Simulator (LAMMPS). Embedded Atom Method (EAM) potential was used for the present study. Pair component of the potential was smoothly stiffened to Ziegler-Bismarck-Littmark (ZBL) potential to account for high-energy collisions between atoms. The successive collision cascades result in continuous damage and a resulting displacement per atom (dpa). Dislocation analysis for dpa of 0.0, 0.5, 1.0 and 2.0 are compared and presented for the two PKA energies.

g0063

Desktop Application for Parallel Defect Analysis & Visualization of MD Simulations of Collision Cascades

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Molecular Dynamics (MD) simulations of collision cascades are an effective way to study the irradiation induced defects in materials. To get reliable statistical results hundreds or thousands of MD simulations of collision cascades are carried out across a wide range of energies generating large scale databases of collision cascades. The tools to analyze and show statistics, patterns and trends in a library of databases can help bring out a lot of insights from these databases. Currently, the tools available for visualizing focus on the analysis and visual inspection of a single simulation. This limits the scope of analysis. We develop a desktop application that analyzes a database of collision cascades in parallel and provides a graphic user interface for complete analysis, visualization and plotting of trends and patterns of the dataset. The application gives a form based graphic user interface to give inputs to analyze the atomic coordinates simulation output file. The analysis involves finding defects, their morphology and size distribution, sub-cascades count and volumes, etc in parallel. Once analyzed different plots, trends, comparisons etc. can be drawn for the dataset quickly through a library view.

g0064

A Machine Learning Workflow to Characterize Defects and Their Morphology in the Atomic Simulations of Crystals

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Irradiation of a material contributes to the formation of defects of various sizes and morphologies such as point defects, dislocations with different Burgers vectors, Lave's phases etc. The defect concentration in addition to the morphology and size distribution decides the microstructural evolution which in turn affects the physical properties of the material. The defect analysis is an important aspect of modeling the radiation damage at atomic scale. The inputs from the atomic scale can then be given to higher scale models like the Kinetic Monte Carlo (KMC). We propose a data-driven approach to analyze the simulation outputs starting from the exploratory unsupervised machine learning which then suggests rules for a deterministic algorithm. The earlier two steps are then used to label the training set for a supervised machine learning model which obviates the need for any deterministic algorithm for later predictions. The final supervised learning model can be used to find defects, their morphology and other attributes. It can be made much more robust to noises and flexible to work with complex simulations such as high-dose irradiation simulations of poly-crystals which are not directly amenable to the deterministic methods.

g0065

Desktop Application for Parallel Defect Analysis & Visualization of MD Simulations of Collision Cascades

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Molecular Dynamics (MD) simulations of collision cascades are an effective way to study the irradiation induced defects in materials and their effects on material properties. To get reliable statistical results thousands of MD simulations of collision cascades are carried out across a wide range of energies generating large scale databases of collision cascades. The tools to visualize and analyze statistics, patterns and trends from a library of collision cascades can help bring out important insights from these databases. Currently, the tools available for visualizing focus on the analysis and visual inspection of a single simulation, computing the properties serially on a single processor. This limits the scope of analysis. We develop a desktop application that analyzes a database of collision cascades in parallel and provides a graphic user interface for complete analysis, visualization and plotting of trends and patterns of the dataset. The analysis involves finding defects, their morphology and size distribution, sub-cascades count and volumes, etc. in parallel. Once analyzed the GUI shows different plots, trends, comparisons etc. for the dataset.

g0066

Inorganic Antiperovskite Nitrides as Photovoltaic Absorbers: Unveiling Excitonic and Polaronic Effects

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Antiperovskite nitrides display promising electronic characteristics for photovoltaic applications, yet they remain underexplored compared to conventional halide perovskites. Due to huge computational demands, their excitonic and polaronic properties have not been rigorously explored. Here, we investigate the optoelectronic properties of these materials, focusing on excitonic and polaronic effects, using state-of-the-art techniques such as hybrid density functional theory, density functional perturbation theory, the Wannier-Mott model, and the Feynman polaron model. We find that these materials possess a suitable band gap, small charge carrier effective masses, and a high dielectric constant. Through the Wannier-Mott model, we observe a low exciton binding energy in these materials, enhancing charge transport properties. Furthermore, weak electron-phonon coupling leads to high charge carrier mobility, indicating their suitability for photovoltaic applications.

g0067

Density Functional Theory Based Study of Structural, Elasto-Mechanical and Electronic Properties of Dy-Filled Skutterudite $DyOs_4P_{12}$ using Full Potential Approach

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We studied the structural, elasto-mechanical and electronic properties of Dy-filled skutterudite $DyOs_4P_{12}$. All the calculations were performed by means of the full potential linearized augmented plane wave method as implemented in Wien2k program package. The exchange-correlation potential was solved with use of the Perdew-Burke-Ernzerhof generalized gradient approximation for solids. The obtained equilibrium lattice constant is in good agreement with the experimental value. The calculated elastic constants show that $DyOs_4P_{12}$ is mechanically stable and brittle in nature. The electronic behaviour of $DyOs_4P_{12}$ is metallic. Theoretical results of elastic and electronic properties are reported for the first time but there are no experimental data available for comparison

g0068

Exploring Electronic and Optical Properties of Heavy Pnictogen Chalcohalide using First-Principles Approach

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In this study, we investigate the electronic and optical property of lower structural dimensional heavy pnictogen chalcohalide. Utilizing first-principles approach, we comprehensively analyze the electronic band structure and optical behaviors of the material. Additionally, we conduct a detailed examination of the dielectric response in both perpendicular and parallel orientations, shedding light on its unique properties. And this study of anisotropic dielectric response which necessitates careful control of preferred orientation in order to achieve efficient charge carrier extraction in device Additionally, within this study, we explore the impact of atomic orbitals on the conduction band minima and valence band maxima by visualizing the density of states.

g0069

BN-DHQ Graphene-like Quantum Dots: Structural and Electronic properties

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In this study, we introduce a quantum dot referred to as boron-nitrogen equivalent deca-hexa-quadrilateral qdot (BN-DHQ), which exhibits similarities to graphene quantum dots but features distinct inner and outer edges. Utilizing ab-initio methods in conjunction with the Gaussian16 code, we have successfully ascertained that all the vibrational frequencies attributed to BN-DHQ are real, confirming its inherent stability. Examination of the electronic attributes of BN-DHQ reveals a significantly large HOMO-LUMO gap of 6.02 eV. This gap stands in notable contrast to its carbon-based 2D counterpart, which possesses a band gap of 2.1 eV. To broaden the spectrum of potential electronic applications, we have purposefully tuned the HOMO-LUMO gap across a range of 2.7 to 3.8 eV. This tuning has been achieved by substituting Fe, Co, and Ni atoms at the outer layers while maintaining almost planar structure. This intentional alteration yields an array of HOMO-LUMO gap values, thereby offering promising potential for electronic and optical device utilization.

g0070

Phase Diagrams of Heisenberg Model in Complex Systems

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Here, we study the ground state phase diagram of J_1-J_2-J_3 Heisenberg model for Mn_{14} cluster with hexagonal symmetry. Using exact diagonalization of s=1/2,1 and 3/2 of 14-site system, we find that the ground state spin changes from 0 to *Ns* with varying J_2, when J_1 = -1 and J_3 < 0. When the system size is doubled (N = 28) the total spin changes almost continuously with J_2. We also study the phase diagram of 2D system or J_1-J_2 model on a three-leg ladder to understand the magnetic properties of Cu_{14} cluster with weak inter-plane interactions.

h) Dielectric, ferroelectric and piezoelectric

h0003

Enhanced Energy Storage Properties of BNT-Based Ceramics Via Cationic Engineering

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Abstract: In this study, the complex-cation $(Mg_{1/3}Nb_{1/3})^{4+}$ substituted lead-free ceramics sodium bismuth titanate ($Na_{0.5}Bi_{0.5}TiO_3$ abbreviate via NBT) synthesized via convential-solid state reaction (SSR) method. The relaxor ferroelectric (RFEs) nature introduce through cationic substitution strategy is adopted in normal ferroelectric (NFE) material. The cation substitution influence structure, ferroelectric, grain growth and dielectric properties has been invested. The cationic content enhances the chemical inhomogeneity and fragmented macroscopic domain into polar-nano regions (PNR's), which increases $\Delta P(P_{max}\text{-}P_r)$ and inhibits grain growth which increases breakdown electric voltage. The good recoverable energy storage density $W_{rec} \approx 1.19$ J/cm^3 obtained in 15 mol% $(Mg_{1/3}Nb_{1/3})^{4+}$ substitution in NBT, as well as thermally stable dielectric constant temperature.

h0004

Effect of A-Site Cation Substitution of Rb^{1+} On Dielectric and Ferroelectric Properties in $Na_{0.2}K_{0.3}Bi_{0.5}TiO_3$

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Abstract: This research work focuses on investigating the effect of A-site Rb^{1+} substitution on $Na_{0.2}K_{0.3}Bi_{0.5}TiO_3$ (RB 0) for 2 mol concentrations of Rb^{1+} (RB 2). Rb-doped NKBT-30 samples are prepared using the conventional solid-state synthesis method. The results obtained from XRD and Raman analysis confirm the existence of a tetragonal phase structure in the samples. The value of T_m is increased from 315 ˚C to 365 ˚C by the substitution of the higher percentage of Rb^{1+}. Dielectric analysis verifies the presence of a distribution of Curie's temperature and enhanced diffused phase transition with an increase in Rb^{1+} doping. The Grain size decreases from 0.473 µm to 0.401 µm due to substitution of Rb. The decrease in the negative strain value with an increase in the concentration of Rb^{1+} confirms the relaxor nature of the crystals. RB2 exhibits the minimum value of remnant polarization (27 µC/cm^2), the maximum value of breakdown field (84 kV/cm), and the minimum value of negative strain, making it a suitable candidate for actuator applications.

h0006

Structural, Morphological And Dielectric Responses Of Zinc Doped Cobalt Ferrite

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Abstract. Zn doped cobalt ferrite with chemical formula $Co1\text{-}xZnxFe_2O_4$ ($x = 0, 0.05$) were prepared by solid state reaction technique followed by reaction sintering at 950°C for 12h. The effect of dopant on structure, microstructure and dielectric property were analyzed. The structural analysis done by XRD spectra revels the formation of cubic structure with Fd-3m space group. The lattice constant value increases slightly after Zn substitution follows the Vegard's law. The calculated value of average crystallite size are 71.74 nm and 74.65 nm for x= 0 and 0.05 respectively. The SEM image clarifies the formation of homogeneous spherical morphology of the synthesized samples. The room temperature dielectric study reveals a decrease in dielectric constant from 23 to 16 after Zn substitution.

h0007

Effect Of Zinc Substitution On Structural, Microstructural And Dielectric Behavior Of Nickel Ferrite

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Abstract. This paper reports the effect of substitution of Zn^{2+} on the structural, microstructural and the dielectric behavior of Nickel ferrite ($NiFe_2O_4$). $NiFe_2O_4$ and $Ni_{0.95}Zn_{0.05}Fe_2O_4$ materials were successfully synthesized using the solid state reaction method. XRD confirms cubic spinel structure of both the samples with Fd-3m space group. The doping increases the values average crystallite size, unit cell parameter and unit cell volume. SEM analysis reveals the decrease in porosity in $Ni_{0.95}Zn_{0.05}Fe_2O_4$ sample. The doped sample shows high dielectric constant and dielectric loss values compared to the undoped sample indicating the enhancement of dielectric properties after doping. The decreasing impedance values with frequency indicate the increasing conductivity with frequency.The dielectric constant values of both the samples are observed to be small compared to the previously reported values indicating the high frequency applications of these samples.

h0008

High Tunneling Electro-Resistance Ratio of a Typical Pt/STO/BTO/SRO Ferroelectric Tunnel Junction

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High Tunneling Electro-resistance ratio (TER) of a Pt/ 20Å SrTiO3 (STO)/16Å BaTiO3 (BTO)/ SrRuO3 (SRO) Ferroelectric Tunneling Junction (FTJ) was investigated. Change in current density and TER with applied bias were studied. A maximum TER of order ~105 was obtained at 0.76V. This high TER is attributed to the unusual potential energy profile of the device at 0.76V, where the barrier height in the ON state (low-resistance state) at BTO/SRO interface almost coincides with the Fermi energy level, giving rise to higher tunneling current density. Transmission probability along with the supply charge flux with incident energy were also studied. Our results are well-consistent with experimental results and hopefully will fuel experimental efforts in studying FTJs with composite barrier.

h0009

Preparation of Cu_2Te/CoTe nanoparticles via rapid microwave-assisted synthesis: A structural, optical, and dielectric study

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Due to various structural and optical properties, metal chalcogenide nanomaterials are favorable candidates for different optoelectronic applications. The current study describes the facile microwave synthesis of Cu_2Te/CoTe nanocomposites with time variation. The crystallinity nature of the materials having hexagonal phases were confirmed from the X-ray diffraction (XRD) analysis. The room temperature Raman spectra showed different vibrational bonds. The field emission scanning electron microscopy (FESEM) images showed nanoparticle structure of the composites, while the energy dispersive X-ray analysis (EDX) spectra identified the elements present in the material. The optical band gap of the nanocomposites is found to be decreasing and a redshift has been observed. The frequency and temperature dependent dielectric study has also been performed. The frequency dependent dielectric constant was found to be decreasing with temperature which enables it for energy storage applications.

h0010

Structure and Dielectric properties of $R_2Ti_2SiO_9$ (R=Nd, Pr)

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In this communication, we report the structure and dielectric properties of monoclinic (C2/m) $R_2Ti_2SiO_9$ (R = Nd and Pr). Both the compounds are isostructural exhibiting relative permittivity in the range of 22-35 and very low loss over a wide frequency range at moderate temperatures. Temperature dependent dielectric studies over 100Hz to 5MHz show that the activation energy for dc conduction is slightly higher in $Nd_2Ti_2SiO_9$ as compared to $Pr_2Ti_2SiO_9$. From the behaviour of the Jonscher power law exponent, it is deduced that the conduction in both the compounds is due to the correlated barrier hopping (CBH) of polarons.

h0011

Dielectric and Magnetoelectric Performance of Alginate Functionalised Ferrite Nanoparticles and Hydrated Salt Incorporated Flexible PVDF Ternary Nanocomposite Fibres

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Magnetoelectric polymer nanocomposites have become highly versatile materials with a wide array of applications, such as ME sensors, energy storage devices, magneto-mechano-electric nanogenerators, and tissue engineering scaffolds. To enhance the functional properties of these composites, a promising approach involves functionalizing ferrite fillers, which improves their interaction with the polymer matrix. In this study, we successfully developed ternary nanocomposite fibres using PVDF loaded with hydrated salt and alginate functionalized ferrite nanoparticles. The nanocomposites incorporating these functionalized ferrite fillers exhibited significantly improved dielectric and magnetoelectric properties. Notably, the ternary nanocomposite fibre containing functionalized nickel ferrite nanoparticles achieved the highest values of dielectric constant (14.7) and magnetoelectric coupling coefficient (18.2 mV cm-1 Oe-1).

h0012

Unravelling the Interplay of Ferroelectricity and Magnetism in Multiferroic compound, $Ba_3HoRu_2O_9$

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The compound $Ba_3HoRu_2O_9$ exhibits multiferroicity and magnetoelectric (ME) coupling. The title compound undergoes long-range antiferromagnetic ordering ~50 K (T_{N1}), followed by another complex magnetic phase transition ~10 K (T_{N2}) with the emergence of co-existing 2nd magnetic phase with ↑↑↓↓ spin-structure. The exchange frustration and strong electronic correlation plays a major role in the distortion of the lattice which might govern ferroelectricity. Here we have shade light on the mechanism of ME coupling which is not explored yet. We demonstrated that Dzyaloshinskii–Moriya interaction arising from two different spin moments of Ru and Ho from 2nd magnetic phase breaks the spatial inversion symmetry and produce local non-zero electric polarization in this compound. However, our combined neutron diffraction and frequency dependance dielectric spectroscopy study suggest that ferroelectric polarization is negligible due to cancellation of random magnetoelectric domains of 2nd magnetic phase. We will discuss the detail mechanism of ME mechanism and domain dynamics.

h0013

Investigation of Multiferroic Property in Fe-modified Bi4Ti3O12; n=3 Layered Aurivillius Ceramics

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Abstract. Here, we report a Fe-modified Bi4Ti3O12 (BTFO); n=3 layered Aurivillius ceramic structural, microstructural, optical, and multiferroic properties. The BTFO Aurivillius ceramics was synthesized by conventional solid-state reaction and purity was confirmed by X-ray diffraction. A Rietveld refinement study revealed that the compound exhibited a predominant orthorhombic structure with the B2cb space group. Structural, microstructural, and UV-Vis spectra analyses were performed to understand the internal lattice arrangements and carrier band structure in detail. The unremitted saturation ferroelectric (P-E Hysteresis) loops at a high field of 45kV/cm were observed. Weak ferromagnetic M-H loops at low temperatures below ≤ 25 K is an indication of a BFTO is a good multiferroic character at low temperature and normal multiferroic at RT.

h0014

Structural, Dielectric, Ferroelectric and Piezoelectric Properties of $BaTiO_3$-$BiFeO_3$ nanocomposites with Enhanced Energy Storage Efficiency

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Abstract. In high-power and pulsed electronic systems, high dielectric permittivity, and substantial energy storage efficiency (η) serve a crucial role for potential applications. Hence, in this work, we propose the synthesis of nanocrystalline composites(1-x) $BaTiO_3$-x$BiFe_{0.95}Mn_{0.05}O_3$ ($0 \leq x \leq 0.3$) via solid state reaction route. The samples are characterized to investigate its structural, morphological, dielectric, ferroelectric and piezoelectric properties. XRD patterns reveal successful loading of magnetic phase in the $BaTiO_3$ matrix. A dense microstructure as revealed from the FESEM micrographs, contributes to the improved dielectric and ferroelectric response of the samples. The low temperature dielectric measurements reveal distinct phase transitions with colossal rise in permittivity values of nanocomposites. The energy storage efficiency rises from 33.8% for pure BTO to 72.5% for the 10 mol% doped nanocomposite. Piezoelectric(d_{33}) coefficients exhibit optimum values for all the samples. The identified characteristics make these nanocomposites a promising candidate for energy storage and ecologically sound pulsed capacitors.

h0015

Comparison of Different Aspect Ratios on Piezoelectric Potential of ZnO, $BaTiO_3$, and PZT-4 Nanorods for the Development of Tactile Sensor

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The present study explores the effect of aspect ratios on piezoelectric potential of three different materials. Three different piezoelectric materials, such as zinc oxide (ZnO), barium titanate ($BaTiO_3$), and standard lead zirconate titanate (PZT-4), have been discussed in the simulation. Among these materials, the ZnO nanorod is receiving a special interest due to its promising piezoelectric properties and biocompatibility. The simulation results show that the ZnO nanorods exhibit greater piezoelectric potential among these three materials due to the lower dielectric constant. This result is in contrast to the fact that the highest piezoelectric coefficient (d_{33}) belongs to PZT and the lowest d_{33} value for ZnO. Further, the simulation study explores the effect of applied pressure on nanorods and the aspect ratio of the nanorods on their piezoelectric performance. These simulation results can be used and optimized for sensitivity and performance in the design of pressure tactile, haptic, and robotics applications.

h0016

Effects Of Doping On Structural, Magnetic and Dielectric Properties Of (Li, Ti, T_m)-doped (T_m~ Cu, Co) NiO Ceramics: A Comparative Study

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Abstract. To understand the effect of Transition Metal ions, Cu and Co doped polycrystalline (Li, Ti) based NiO ceramics (abbreviated as LTNO_Cu and LTNO_Co) have been synthesized by solid state reaction method with optimum (Cu, Co ~ 0.02%) dopant concentration and later characterized by various experimental techniques. The crystallographic structure and phase-identification of sample are characterized by x-ray diffraction. From Rietveld refinement final stoichiometry is found to be $Li_{0.3}Ti_{0.02}Co_{0.02}Ni_{0.66}O$ and $Li_{0.3}Ti_{0.02}Cu_{0.02}Ni_{0.66}O$ with $Fm\bar{3}m$ space group. SEM microstructural analysis reveals distinct domain formation inside the grain for LTNO_Cu (~ 0.17 μm) and LTNO_Co (0.44 μm), respectively in contrast to ~0.025 μm for pure (Li, Ti) based NiO ceramics. Magnetic transition also decreases with additional doping of Cu and Co.Dielectric properties are measured as a function of frequency (20Hz-1MHz) in temperature range (2K-300K). Giant dielectric response ($\varepsilon' \sim 10^3$) is observed for both the samples. IBLC mechanism based on domain and domain boundary having electrically heterogenous properties is used to explain resulting behavior. Electrical circuit deconvoluted from observed behavior is thus described by series connection of parallel equivalents of resistance and constant phase element of domain and domain boundary, respectively.

h0017

Dual band Terahertz Microstrip Patch Antenna for Satellite Communication Applications

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Abstract. The investigation of terahertz frequency ranges has become crucial due to the rising need for ultra-fast wireless communication technologies. The performance of the theoretically designed high-frequency patch antenna working at an astonishing frequency in the terahertz range is analysed. The voltage standing wave ratio (VSWR) of 1.0043 at 1.98 and 1.22 at 2.46 THz operating frequencies are improved by the suggested patch antenna utility for the dual band frequencies of -35.11dB at 1.98 THz and -23.04 dB at 2.46 THz. High frequency structure simulation software (HFSS) is used to study the associated characteristics of this antenna. Due to its small size, the antenna may be easily integrated into a variety of products and wireless communication systems, with the potential to revolutionist the next-generation 5G and beyond.

h0018

Impact of C doping on the structural, dielectric, and electric properties of MoO_3

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The introduction of doping in transition metal oxides, like Molybdenum oxide (MoO3), brings about notable structural modifications that play a crucial role in fine-tuning their properties and broadening their range of practical applications. MoO3 nanostructures were fabricated during hydrothermal technique and the substitutional doping of carbon (C) were done using post calcination process. To investigate the dielectric and electric properties of MoO3 and C doped MoO3 at different (0.5, 1, 2, 4, 8, 10, 12 and 15 wt%) weight percentages were obtained. The structural analysis of the samples was conducted using X-Ray Diffraction (XRD), while Fourier Transform Infrared spectroscopy (FTIR) was utilized to determine the chemical composition. For investigating the dielectric properties of both undoped and carbon-doped MoO3 nanostructures, dielectric spectroscopy (DS) was employed over a wide frequency range of 102-106 Hz at room temperature. The dielectric study revealed significant alterations in dynamics, including changes in dielectric constant, dielectric loss tangent, capacitance, and electrical conductivity.

h0019

Studies of Structural and Ferroelectric Behaviour of Eco-friendly $K_{0.5}Bi_{0.5}TiO_3$ Ceramics

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Abstract. In this article, we reported successful preparation of potassium bismuth titanate (KBT) ceramics by sol-gel technique. Structural and electrical properties were investigated with variation of temperature. X-ray diffraction study and the Rietveld refinement patterns revealed the P4mm tetragonal phases of the samples. Temperature dependence of leakage current density with electric field was observed from 20-180 ^oC. The P-E loop traces demonstrated good saturation in the sample curves. The saturated P-E loop curves helps in increasing the applied electric field, which improves ferroelectric characteristics.

h0020

Structural, morphological and dielectric properties of Mg-doped ZnO nanoceramics prepared by sol-gel method

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$Zn_{1-x}Mg_xO$ (x=0, 0.15) ceramics were successfully synthesized by sol-gel method. Structural analysis was performed by XRD confirming phase purity and hexagonal wurtzite structure. The change in lattice parameters, and bond length for Mg doped ZnO sample indicates Mg2+ ions incorporation in ZnO lattice. Crystallite size is decreased with the increase in 'Mg' content. SEM analysis reveals that grains of the samples are homogeneously distributed. The dielectric constants (εr), dielctric loss (tan d) were studied as the function of frequency and composition. Investigation of dielectric properties of samples revealed that the value of dielectric constant at low frequency is large while in the higher frequency regime, a frequency independent behavior was observed.

h0021

Negative Capacitance Effect in Silica-doped Copper Oxide

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A comprehensive study of the effect of ball-milled processed non-magnetic Si-doping in cupric oxide (CuO) has been discussed in this literature. Different experimental techniques like x-ray diffraction, dielectric spectroscopy, magnetic measurements have been performed to find the effective changes observed in CuO. This small quantity of substitution brings out changes in crystal structure, transport conduction, and magnetic transition. Unique inductive loops and negative capacitance characteristics was observed in the complex impedance plot at low frequency. Analyzing impedance spectroscopy, we adopt surface polarization model based on the assumption of large electric and ionic charge accumulation at the external contact interface. The inductance element in the equivalent circuit is the result of the delay of the surface voltage and depends on the kinetic relaxation time. While the substitution of Cu by Si, the antiferromagnetic transition decreases to ~216 K (T_{N1}).

h0022

Impact of Mg^{2+} Ions Doping on the Structural and Dielectric Properties of Gd_2FeCrO_6

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The structural, microstructural and dielectric properties of double perovskites, Gd_2FeCrO_6 and $Gd_2FeCr_{0.75}Mg_{0.25}O_6$ are reported. The structural analysis of the compounds fabricated using sol-gel method is performed by powder XRD technique, which revealed the monoclinic crystal structure. The scanning electron microscopy studies showed nearly spherical grains for both perovskites with the average grain size of about 100 - 150 nm. The impedance and dielectric constant as a function of temperature (30-300 ^oC) and frequency (100 Hz-1MHz) have been investigated. The temperature dependent dielectric constant measurements suggested the time relaxor behaviour of these materials. The impedance was found to be decreased with increase in temperature, showing negative temperature coefficient of resistance. The Gd_2FeCrO_6 compound has larger impedance and lower dielectric constant with respect to doped perovskite, $Gd_2FeCr_{0.75}Mg_{0.25}O_6$ compound. By these findings, it may be concluded that these materials have potential applications in high temperature electronic devices.

h0023

Structural, Optical and Dielectric Properties of $CaZrO_3$ Ceramic Synthesized by Solid-State Method

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In the present paper, single-phase $CaZrO_3$ ceramic is synthesized by solid-state reaction method and characterized by using X-ray diffraction, scanning electron microscopy techniques. Analysis of electrical properties is conducted by impedance spectroscopy measurements in frequency range 10 kHz to 5 MHz at room temperature. The higher values of dielectric constant at the lower frequencies are explained on the basis of the Maxwell–Wagner (MW) polarization model. The variation of impedance as a function of frequency revealed the relaxation behaviour of this material. This property makes it a suitable candidate for energy storage and electrical devices.

h0024

Structural and Impedance Spectroscopic Studies of Ca Substituted Lead Titanate Ceramics

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The Ca substituted $Pb_{1-x}CaxTiO_3$ (x=0.00,0.01,0.03,0.05,0.07,0.1) ferroelectric materials were synthesized by solid state reaction method. The X-ray diffraction studies confirm that all samples belong to tetragonal structure. The variations of lattice parameter and anisotropy constant are observed with increasing Ca concentration. The temperature dependence of dielectric constant at different frequencies for un-substituted and Ca substituted Pb1-xCaxTiO3 are measured. The dielectric dispersion is observed for all samples. From impedance spectroscopic data the Relaxation times (τ), activation energy (Ez), Grain resistance (Rg) and Grain capacitance (Cg) were measured. Cole-Cole plots confirms that non-Debye kind of relaxation process in the material.

h0026

Structural and Dielectric Study of the Potassium Sodium Niobate/ Polyvinylidene Fluoride Nano-composite Thick Films

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Abstract: Potassium sodium niobate/polyvinylidene fluoride (KNN/PVDF) nanocomposite thick films were synthesized using the solution casting method. Investigation of structural, surface morphology, and dielectric characteristics provided a clear picture of the impact of KNN as filler in the PVDF matrix. Raman spectroscopy showed that the beta fraction (β) is found to be maximum (71%) in 10 wt.% KNN loaded film and decrease further with an increase in loading concentration due to agglomeration whose influence is also seen on dielectric properties. 10 wt. % KNN-PVDF composite had the highest dielectric constant of 18 at 100 Hz.

h0027

Investigation of structural and glassy behaviour of 0.90 $BaTiO_3$-0.10 $Bi(Mg_{2/3}Nb_{1/3})O_3$ Relaxor.

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0.90 $BaTiO_3$(BT)-0.10 $Bi(Mg_{2/3}Nb_{1/3})O_3$ (BMN) solid solution is synthesized by conventional solid state reaction method. Reitvelt refinement of the room temperature X-Ray Diffraction pattern conveys a tetragonal structure with P4mm space-group which is further confirmed by the Raman Spectroscopy. Dielectric properties of the 0.90BT-0.10BMN ceramic as a function of temperature (173K-473K) have been analyzed at different applied frequencies. The glassy behaviour of the ceramic has been analyzed by applying Vogel-Fulcher relationship to the variation of T_m (temperature related to the maximum permittivity value) with frequency. The Polarization-Electric field loop has been taken around the break down field which shows a slim hysteresis loop with 82% energy storage efficiency.

h0028

Investigation of Dielectric Properties of Corundum Type Antiferromagnet: $Co_4Ta_2O_9$

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In the current scenario of condensed matter physics, it is essential to explore the advanced multifunctional materials where one can tune their properties by external means like temperature, pressure, electric and magnetic field etc. Co4Ta2O9 (CTO) is one of the interesting magnetoelectric materials. It exhibits interesting magnetoelectric coupling across its antiferromagnetic transition. But there is not enough effort made to explore the dielectric behavior of this material. Herein, we have investigated the structural and temperature dependent dielectric properties of polycrystalline CTO well above its magnetic ordering temperature. We have synthesized the polycrystalline sample of CTO by solid state reaction route. The room temperature (RT) structure is investigated by x-ray diffraction (XRD) technique. The Rietveld refinement of RT XRD patterns confirmed that CTO crystallizes in pure trigonal phase (P-3c1). A clear frequency dispersion is observed near 105 K, which was not explored before. Comprehensive complex modulus analysis has been done to study the different contributions to the observed relaxation.

h0029

Studies of Dielectric Behavior of Ho^{3+} Doped La_2NiMnO_6

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Double perovskite La_2NiMnO_6 (LNMO) and holmium (Ho) doped LNMO were synthesized via solid state route. The obtained PXRD patterns confirmed the formation of a monoclinic crystal structure with space group P21/n. Through temperature-dependent and frequency-dependent dielectric studies, it was observed that the introduction of holmium as a dopant led to a reduction in the dielectric constant and dielectric loss compared to pure LNMO. This phenomenon was attributed to modifications in the charge states of Ni and Mn ions brought about by the incorporation of holmium into the lattice. Impedance analysis revealed an increased conductivity upon Ho substitution, indicating the influence of holmium on electrical conductivity.

h0031

Effect of Monovalent and Divalent Doping Ions on Structural, Optical and Electrical Properties of TiO2 Nanoparticles

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In this study pure anatase TiO_2 nanoparticles and its derivatives [i.e. ($TiN_{0.007}O_{1.993}$), ($Ti_{0.998}Cu_{0.002}O_2$) and ($Ti_{0.998}Cu_{0.002}N_{0.007}O_{1.993}$)] were synthesized by sol-gel technique. Structural, optical and dielectric properties of TiO_2 and its derivatives were investigated using X-ray diffraction (XRD), UV-visible spectroscopy and dielectric spectroscopy measurement respectively. XRD data revealed that all the samples have pure anatase phase having tetragonal structure with space group of I41/amd and other crystallite size of TiO_2 and its derivatives were found in the range of 10-15 nm, calculated by Scherrer's formula. The band gap of TiO_2 and its derivatives has been observed to be reduced from 3.20eV to1.90 eV as confirmed by UV-visible spectroscopy. Cu and mono doped TiO_2 nanoparticles effectively modify dielectric behavior and conductivity behavior of all the samples understudy.

h0033

Tailoring the Structural, Dielectric and Magnetic Properties of YCrO3 Perovskite via Fe Doping

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Abstract. The sol-gel synthesized Fe-doped YCrO3 have been investigated for its optical, electrical, dielectric and magnetic properties. We utilized various techniques, including X-Ray Diffraction (XRD), Rietvield Refinement, VSM and Temperature-Dependent Dielectric Spectroscopy for a comprehensive study of this Transition Metal Oxide (TMO). Further, we examined M-T and M-H properties and determined the magnetoelectric coupling coefficient. The origin of the observed magnetoelectric coupling effect can be attributed to the magnetocrystalline anisotropy and microstrain. According to the results obtained, the excellent electrical and magnetic properties of Fe doped YCrO3 are promising for high-end spintronics study.

h0034

The Effect of Ionic Radius on the Multifunctional Properties of Lead-Free $SrBi_2Nb_2O_9$ Ceramic Materials

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Abstract. The primary goal of this work is to investigate the effect of dopant ionic radius RE^{3+} (RE = Pr^{3+}/Eu^{3+}/Dy^{3+}/Sm^{3+}) cation on the structural and physical aspects of SBN-based perovskite materials. X-ray diffraction patterns assure the orthorhombic structure of the produced samples. It was observed that the lattice parameters exhibited a positive correlation with the ionic radius of the dopant cation as realized from reduced lattice strain, and improved crystallinity. The morphological changes in tune with that of ionic radii were assured from the SEM study. The ionic radii of the dopant had impacted electronic transitions and hence the optical properties of SBN ceramics. The magnetic anisotropy was induced due to the ionic radius of the dopant leading to RTFM behavior. The influence of dopant content on mechanical properties has been perceived from microstructure engineering. The existence of a dopant in the SBN matrix maneuvered the multifunctionality of the material.

h0035

Investigation of High-Temperature Dielectric Relaxation and Electric Conduction Mechanisms in $LaCoO_3$ Modified $Na_{0.5}Bi_{0.5}TiO_3$ System

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The solid solutions of $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) with $LaCoO_3$ materials having general chemical composition (1–x) [$Na_{0.5}Bi_{0.5}TiO_3$] + x [$LaCoO_3$] with x= 0.05, 0.10 and 0.15 (abbreviated as LCNBT5, LCNBT10 and LCNBT15) were fabricated by using the sol-gel technique. The findings demonstrate that all the samples exhibit two dielectric transitions: firstly, a frequency-dispersive shoulder at a lower temperature (T_s) around 425 K - 450 K which is associated with polar nanoregions (PNRs), and secondly, from ferroelectric to paraelectric transition at Curie Temperature (T_c) approximately between 580 K-650 K. The impedance analysis reveals the negative temperature coefficient of resistance behavior of the specimens. The oxygen vacancies created with the addition of $LaCoO_3$ in the $Na_{0.5}Bi_{0.5}TiO_3$ ceramics are responsible for the relaxation and conduction processes, and the charge carrier is largely made up of doubly ionized oxygen ion vacancies.

h0036

Structural and optical properties of ZnO nanorods derived from sol-gel method

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Abstract. Nanostructured zinc oxide (ZnO) is a promising material for several applications in different disciplines. Herein, we have synthesized ZnO nanorods by utilising a simple sol-gel method in which zinc acetate was taken as the starting material. The crystallinity, phase formation, and crystallite size of the nanostructures were examined using X-ray diffraction (XRD). The morphology of the produced nanostructures has been studied using field-emission scanning electron microscopy (FE-SEM). A rod-like morphology having average length and diameter were found to be 600 nm and 60 nm, respectively. The results of the Energy Dispersive X-ray (EDX) reveal high purity of the stoichiometric ZnO nanoparticles. UV-Vis spectroscopy data reveal the absorption of UV radiation corresponding to the band gap of 3.5 eV as estimated by using Tauc's plot.

h0037

Structural and Dielectric Properties of Sc Doped 0.94NBT-0.06BT Lead Free Ceramics

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Lead free piezoelectric ceramics $0.94Na_{0.5}Bi_{0.5-x}Sc_xTiO_3$-$0.06BaTiO_3$ (x = 0.0, and 0.05) doped with Scandium (Sc) were prepared by a standard solid state reaction. Structural properties of samples were studied using powdered XRD and Raman spectroscopy. The coexistence of rhombohedral and tetragonal phases in both ceramics is observed from the XRD. Dielectric measurements and analysis were performed from room temperature to 450 °C at various frequencies. The relaxor nature of the ceramics was observed with the diffusive phase transition at the dielectric maxima. The substitution of Scandium in NBT-6BT has increased the transition temperatures T_d and T_m.

h0038

Exploring The Correlation Between Morphology And Magnetodielectric Properties In $KBiFe_2O_5$-$CoFe_2O_4$ Composite

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Abstract- In the age of machine learning and artificial intelligence, there is a need for a new multifunctional device that is lighter, faster, and more energy efficient. Due to the fascinating multiferroic characteristics of $KBiFe_2O_5$ and its composite with ferrite, it has attracted much attention, making it a viable material for various device applications, including sensors, actuators, memory, and other technological ones. In this study, we report the synthesis of (1-x)$KBiFe_2O_5$-(x)$CoFe_2O_4$ composite using a citric-assisted sol-gel method. X-ray diffraction (XRD) data confirms the phase formation of the prepared composite. Field scanning electron microscopy (FSEM) of the prepared composite reveals the presence of both types of grains of the parent material ($KBiFe_2O_5$ and $CoFe_2O_4$), confirming the successful formation of the composite phase. Magnetodielectric measurement confirms the enhanced coupling in the composite as compared to $KBiFe_2O_5$, which is attributed to the addition of ferromagnetic $CoFe_2O_4$.

h0039

Structural and Dielectric Properties of $LaFeO_3$ Orthoferrite Ceramics

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Abstract. $LaFeO_3$ orthoferrite perovskite is synthesized by conventional solid-state reaction method. The structural properties of the sample is studied through X-ray Diffraction (XRD) which indicates an orthorhombic structure with lattice parameters "a" =5.5560 Å, "b" =5.5650 Å and "c" =7.8620 Å at room temperature. The Dielectric constant(ε_r)and tangent loss($\tan\delta$) of the above ceramic compound are studied over a temperature range 25^0C -380^0C with different frequencies. The different dielectric

values with frequency and temperature have been provided.

h0040

Study of Phase Formation and Electrical Properties of Double Perovskite Y_2NiMnO_6

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Abstract: The double perovskite oxide Y_2NiMnO_6 has been synthesized using the conventional ceramic route. The crystal structure of the Y_2NiMnO_6 was confirmed to be monoclinic in the space group P2_1/c (14) through Rietveld refinement. The electrical properties have been studied in the frequency range of 20Hz - 2MHz and temperature range of RT - 600°C. The AC conductivity behavior of the sample shows a transition from an insulator/semiconductor to a metal-like material. Moreover,

the material exhibited a transition from positive to negative permittivity at 210°C. This transition is attributed to the change in electrical characteristics of the material from a capacitor to an inductor.

h0041

Studies on Microstructural and Electrical Properties of BST Lead-Free Piezoceramics

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Abstract: It is the prime interest in scientific society to enhance the capacitor's energy density and voltages for applications in the fast-growing industries of automotive, microelectronics, renewable energy production and transmission, medical, etc. In this work, we report a systematic study on the microstructural, dielectric, and ferroelectric properties of lead-free piezoelectric materials $(Ba_{1-x}Sr_x)TiO_3$ using techniques such as XRD, FE-SEM, impedance analyzer, and ferroelectric loop tracer. The piezoceramics samples were fabricated using a conventional solid-state reaction route. The microstructures of all prepared samples are uniform and dense, with a small number of pores. Phase transition temperature was shifted toward lower temperature at low frequency. Ferroelectric properties appraised by the P–E loop have been traced. The investigated data of P-E loops reveals that the different values of remnant polarization are primarily owing to leakage current contribution at larger electric fields. These properties promise BST to be applicable in Pb-free tunable devices and very suitable for pyroelectric materials working at the dielectric bolometer mode.

h0043

Impedance studies of $Ba_{0.96}Ca_{0.04}Ti_{0.96}Mn_{0.04}O_3$ Solid Solution

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Abstract. Polycrystalline samples of $Ba_{0.96}Ca_{0.04}Ti_{0.96}Mn_{0.04}O_3$ (BCTM) were synthesised using solid state reaction route. Impedance spectroscopy data reveals that the grain boundaries are more resistive than grains. The activation energy of BCTM sample calculated from Z``, M`` and ac conductivity data was found to be almost equal (≈1.05 eV) implying that the conduction and relaxation processes occurring in the samples can be attributed to same type of charge carriers. The activation energy ≈1.05 eV is indicative of the presence of doubly charged oxygen vacancies. A single depressed semicircle in Nyquist plots was observed indicating the non Debye type behaviour and the overlapped contribution of grains and grain boundaries. The increase in the value of conductivity exponent 'n' (and n <1) with temperature suggest electrical conduction to be dominated by non - overlapping small polaron tunneling.

h0044

Impact of ac Frequency on Polarization in Sn-Substituted NBT-BT Ceramics Near MPB

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Abstract. The present work focuses on the dependence of polarization (P) dynamics on the sweep rate of external alternating current (ac) on the electric field (E) of Sn-doped 0.94 NBT - 0.06 BT near at MPB region. The structural and ferroelectric properties of Sn-doped NBT-BT ceramics were investigated. X-ray diffraction patterns confirmed the perovskite structure with a pseudo-cubic phase in Sn-substituted NBT-BT ceramics. Polynomial fits were applied to investigate the systematic variation of remnant and saturation polarization with frequency. The frequency dependence of P-E loops indicates that decreasing remnant and saturation polarization with increasing frequency suggests intrinsic polarization mechanisms due to domain wall dynamics and domain switching behavior. These findings lay the foundation for future investigations into temperature-dependent dielectric and further frequency-dependent ferroelectric studies.

h0046

Thermally Stimulated Spontaneous Current Spectra In Pristine And 100 MeV Ni Ion Irradiated PET/0.8PHB Polymer Liquid Crystals

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Abstract. Thermally stimulated spontaneous (TSS) current spectra, of the order of pico amperes (pA), of pristine and 100 MeV Ni-ion irradiated PET/0.8PHB polymer liquid crystals were investigated. TSS current spectra of these materials studied with various electrode materials (M:P:M) viz. Bismuth(Bi), Aluminium(Al) and Gold(Au), with different heating rates (2^0C, 4^0C and 6^0C/minute). The material was irradiated with fluence 9.37×10^{11} ions/cm^2 by 100 MeV Ni - ions in the temperature range from 38^0C to 250^0C at IUAC, New Delhi. TSS current spectra varies linearly with temperature in the temperature region from 38^0C to 140^0C. It is also clear from the experimental data, that a decrease in the magnitude of TSS currents with increase in heating rate and even changes the polarity with higher heating rates.

h0047

Magnetodielectric and Magneto Photocatalytic Study of $BaFe_{12}O_{19}$ Hexaferrite

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The room temperature multiferroic $BaFe_{12}O_{19}$ (BFO) hexaferrite is synthesized by conventional solid state reaction route. The prepared sample is characterized for its multifunctional properties like magnetodielectric (MD), photocatalytic and magneto-photocatalytic properties. The room temperature (RT) X-ray diffraction results reveal that BFO crystalizes as hexagonal symmetry with space group *P*63/*mmc*. The RT isothermal MD results illustrate that MD increases with increasing magnetic field till 11 kOe and then starts decreasing with further increasing the magnetic field. The maximum MD (~1.58%) is observed around 11 kOe. The photocatalytic activity of magnetic field poled and unpoled BFO is performed on methyl green (MG) dye in sunlight. The 3 mg per 5ml of $20mg/L^{-1}$ solution of poled and unpoled BFO is explored by ultra violet visible (UV-VIS) spectroscopy. A significant enhancement (~14 %) of dye degradation is observed in the magnetic field poled BFO within 160 minutes exposure of sunlight. These results illustrate that magnetic field poled BFO has better dye degradation capability for MG dye. This enhancement in catalytical properties by magnetic field will be a most promising technique for waste water treatment.

h0048

Synthesis And Characterization of Strontium Doped Barium Titanate by Using Solid State Reaction Route

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Abstract. Engineering of lead-free ceramic materials with promising dielectric and piezoelectric properties is an innovative way for their multifunctionality. Herein, we report the synthesis of strontium ion (Sr^{2+}) doped $BaTiO_3$ (BT) to realize $Ba_{1-x}Sr_xTiO_3$ (x = 0, 1 and 15 wt%) ceramic nanoparticles by a simple solid state reaction route. The synthesized samples were characterized by x-ray diffraction technique (XRD), field emission scanning electron microscope (FE-SEM), Fourier transform infrared spectroscopy method and impedance analyzer. Tetragonal phase of BT has been revealed by XRD technique. Additionally, a systematic shift of the peak positions, with increased amount of Sr doping, towards higher angle side confirms Sr^{2+} doping at Ba^{2+}-site. FESEM images show the spherical particle having relatively smaller size (100 -125 nm) for x = 0 sample. On Sr doping, particle size is found to increase (125 – 150 nm) having more or less similar morphology as for x = 0. Impedance analyzer results reveal an increase in dielectric constant with Sr^{2+} doping in lower frequency range. The observed results suggest its application in electromechanical nanogenerator and energy storage devices.

h0049

Dielectric studies of MgCu2O3 compound

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In the present work, we present the dielectric studies of the $MgCu_2O_3$ compound, synthesized by solid-state reaction. The sample was characterized by x-ray diffraction (XRD). The XRD results show that the synthesized sample is of güggenite α-type which is iso-structural with $CaCu_2O_3$. The dielectric properties were carried out by impedance spectroscopy which shows the frequency dependence of relative permittivity for the $MgCu_2O_3$ compound. The value of relative permittivity is found to be ~450 at 100 Hz frequency. The tangent loss spectrum shows that multiple relaxations may exist in the sample. The sample morphology was examined by field emission scanning electron microscopy (FE-SEM).

h0050

B-site doped $GdInO_3$ system: Structure and Tunability of Electrical Behaviour

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Rare earth based, ABO_3 hexagonal class of materials possesses structural features conducive to introduction of geometric ferroelectricity. With this motivation, the structural tunability of hexagonal ABO_3 is explored by synthesizing B-site tailored $GdInO_3$ series by gel combustion technique and annealed at four different temperatures to explore their extensive structural and electrical behaviour. Phase relations were strikingly different despite similar tolerance factors. The temperature was found to have tremendous bearing on the phase relations. The system exhibited rich phase relations consisting of metastable C-type modifications, hexagonal, orthorhombic and biphasic modifications. Raman spectroscopy was employed to analyse the structural changes at local level to augment the XRD data e.g., in $GdIn_{1-x}Fe_xO_3$ ($0.0 \leq x \leq 0.1$), a general shrinkage of the hexagonal lattice due to substitution of a smaller ion at Fe^{3+}-site was observed but an apparent dilation of Gd-O bond was

exhibited by Raman spectroscopy. $GdIn_{1-x}Fe_xO_3$ system showed systematic increase in dielectric constant over 10 orders of magnitude at 250 °C with Fe-content. Dielectric constant and tan δ show steep increase with temperature for Fe-rich system.

h0051

Effect Of Sintering Temperature On The Structural, Morphological, And Ferroelectric Properties Of La Substituted Barium Hexaferrite, $Ba_{(1-x)}La_{(x)}Fe_{12}O_{19}$, (x=0.25 and 0.30)

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Abstract. The La substituted M-type Barium hexaferrite, $Ba_{(1-x)}La_{(x)}Fe_{12}O_{19}$, (x=0.25 and 0.30) were synthesised using ball milling followed by heat treatment at 1150˚C and 1300˚C and the influence of sintering temperature as well as doping were presented. X-Ray diffraction, FESEM, and ferroelectric measurements were performed to study structural, morphological, and ferroelectric properties of the prepared sample. Rietveld refinement on the X-Ray diffraction measurement reveals the formation of single phase magnetoplumbite structure of barium hexaferrite only for the samples sintered at 1300˚C. Secondary phase along with major magnetoplumbite structure was observed for sample sintered at 1150˚C. Hexagonal plate like grains with different sizes were observed and sample sintered at 1300˚C show large size grains. Porosity observed to decrease with La doping. Ferroelectric studies show leaky P-E loop for low temperature (1150˚) sintered samples. Also, with doping withstanding of electric field observed in the same. However, ferroelectric property suppressed for samples sintered at 1300˚C.

h0052

Effect of of TeO_2 on the glass formation, thermal, structural and optical properties of Li_2O-GeO_2-SiO_2 glasses

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Abstract: The glasses under investigation have been prepared by melt quenching technique. The amorphous nature of the prepared glasses is confirmed by X-ray diffraction studies. Thermal stability was analyzed by DSC. EDS, FTIR spectroscopic studies were employed to investigate the structure of the prepared glasses. Amongst all the samples glass forming ability and thermal stability is high for the glass doped with 5 mol % of TeO_2. The UV–vis spectra in the range of 200–1200 nm wavelength for the proposed glasses were recorded. Based on the absorption spectra, band gap of optical energy (E_g) has been evaluated and the highest value is obtained for Te5 sample (3.41 eV). The analysis of these spectroscopic investigations reveals that the glass doped with 5 mol % of TeO_2 is suitable for dielectrics and optical fibers.

h0054

Investigation of Electrical, Dielectric, and Magnetic properties of $(BiBa)(FeMn_2)O_8$

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A new compound of chemical formula $(BiBa)(FeMn_2)O8$ was prepared by a solid-state reaction method. X-ray structural studies confirm orthorhombic unit cell of the compound. Surface morphology comprises non-uniform granular structure in which grains are of polyhedral type. Average grain size was found to be 0.6 µm. Room-temperature magnetic data displays ferromagnetic hysteresis loop with high value of effective magnetic moments. The dependence of dielectric constant and loss tangent at different frequencies (1 kHz -1 MHz) were measured using LCR meter on rise of temperature from room temperature to 500 ºC. The dielectric constant increases on rise of temperature due to Maxell-Wagner polarization and the loss tangent displays similar behavior. A low value of loss tangent is obtained at higher frequencies, which paves the way for the application of the compound in high frequency devices.

h0055

Electrical Properties of Sputtered AlN/Si (111) for Piezoelectric MEMS Applications

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Abstract: Aluminum nitride (AlN) thin films are reactively sputtered on Si (111) substrate at low temperature (< 400 °C) for piezoelectric-based MEMS applications. The prepared wurtzite-AlN film shows polycrystalline nature with (002) preferred orientation. The Metal-Insulator-Semiconductor (MIS) structure is fabricated to study the electrical properties of AlN thin films. The leakage current by the *I-V* measurement was as low as 1.4 pA. The dielectric constant of the AlN films increased from 10.8 to 19.8 as the substrate temperature increased. The trapped charges are crucial in controlling the electrical characteristics and low interface trap density (6.72×10^{10} cm^{-2} eV^{-1}) observed for the sputtered AlN grown at a substrate

temperature of 300 °C. This study on the structural and electrical properties of AlN/Si (111) at low substrate temperature is compatible with the complementary metal oxide semiconductor (CMOS) process for constructing piezoelectric-based microelectromechanical systems (MEMS) devices for various applications.

h0057

Investigation of Structural and Ferroelectric Properties of Titanium Doped $AgNbO_3$

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Polycrystalline Ti4+ doped AgNbO3 sample was prepared using solid state reaction. The X-ray diffraction studies indicated that the sample stabilized in orthorhombic structure with Pmc21 space group. The scanning electron microscope images revealed that the grains were in cube type shape. The ferroelectric polarization hysteresis loop showed a remanent polarization of 3.9 µC/cm2. The FTIR spectrograph showed a band of vibrational modes corresponding to Nb-O bonds from 500 cm-1 to 1000 cm-1.

h0058

Graphene Based PVA/PVP Composite Films Showing Enhanced Dielectric Properties & AC Conductivity Behaviour

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The dielectric and AC conductivity properties of Polyvinyl Alcohol (PVA)/Polyvinyl Pyrrolidone (PVP) blend Graphene nanocomposites have been investigated in this study. The incorporation of graphene nanoparticles into polymer blends offers the potential to enhance the electrical and mechanical properties of the resulting nanocomposites. In this work, PVA and PVP were selected as matrix polymers due to their complementary characteristics in terms of mechanical strength and flexibility. Dielectric analysis revealed a substantial increase in the dielectric constant of the nanocomposites with the addition of graphene. The AC conductivity measurements exhibited a notable enhancement in electrical conductivity compared to pristine PVA/PVP blend, ascribed to the percolative conductive networks formed by well-dispersed graphene nanoplatelets. The study elucidates the synergistic effects of PVA/PVP blend and graphene nanoplatelets on the dielectric and AC conductivity behaviors of nanocomposites. These findings provide valuable insights into tailoring the electrical properties of polymer blend graphene nanocomposites, holding promise for applications in flexible electronics, capacitors, and energy storage devices.

h0059

Investigation of Structural, Dielectric and Magnetic Characteristics of La Doped CuO Multiferroic

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Abstract: In this manuscript, we report room temperature structural, optical, microstructural, magnetic and dielectric properties of solid-state reaction method synthesised CuO and $Cu_{0.995}La_{0.005}O$ ceramics. Doping of La in CuO leads to the evolution of dense and compact microstructure with reduced porosity. Due to noticeable differences in the ionic radii of La^{3+} (1.03Å) and Cu^{2+} (0.73Å), La doping creates vacancy defects which induces considerable strain in the CuO lattice leading to a decrease in the lattice parameters and cell volume. However, both ceramics processes exhibit a similar monoclinic structure with C2/c space group. Detailed characterization using Raman and FTIR and XPS spectroscopy confirmed the incorporation of the La^{3+} in CuO lattice. Interestingly, doping with La significantly increases the dielectric constant of CuO and leading to a decrease in leakage current. The observed increase in dielectric constant can be attributed to the presence of a dense microstructure and strain/distortion in the CuO lattice after La doping. Furthermore, it can be observed that the bandgap of $Cu_{0.995}La_{0.005}O$ ceramics decreases which is attributed to increased vacancy defect concentration which leads to the creation of intermediate dopant energy levels within the bandgap of the CuO matrix. that creates intermediate dopant energy level within bandgap of CuO matrix. Furthermore, improvement in magnetic and dielectric properties is also discussed and correlated with the grain size in La-doped CuO.

h0060

Modification of $(K_{0.5}Na_{0.5})NbO_3$ in Ternary [0.94 $(Bi_{0.5}Na_{0.5})Tio_3$-0.06$Ba_{0.85}Ca_{0.15}Ti_{0.9}Zr_{0.1}O_3$] Lead Free Piezoceramics

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Abstract: [(0.94−x) $(Bi_{0.5}Na_{0.5})$ TiO_3-0.06$Ba_{0.85}Ca_{0.15}Ti_{0.9}Zr_{0.1}O_3$]-x($K_{0.5}Na_{0.5}$) NbO_3 lead free piezoceramics were prepared by using solid state reaction method. The influence of KNN on structural, microstructural, electrical properties of the polycrystalline NBT-BCZT-KNN samples were studied. Powder X-ray diffraction (PXRD) results shows that KNN dissolved into NBT-BCZT samples form a new solid solution. NBT-BCZT-KNN samples shows pure perovskite structure with a Rhombohedral phase structure. From the dielectric measurement, the maximum temperature (T_m) and depolarization temperature (T_d) are 310 ◦C and 140 ◦C. Relaxation behaviour are observed at the ratio of x=0.06 KNN. Dielectric constant (ε_r) increased; maximum temperature (T_m), depolarisation temperature (T_d) and density decrease with increasing KNN content.

The ε_r in the range of 1019 -3700, Tc~310 ℃ and dielectric loss is 0.015. In As a result, [(0.94−x) BNT–0.06 BCTZ]-x KNN ceramics are a promising candidate material for the mobile electronic device**.**

h0061

Dielectric and Raman Spectroscopic Properties of High Dielectric and Metamagnetic Eu_2CoMnO_6 Perovskite

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Monophasic and polycrystalline Eu_2CoMnO_6 is synthesized, and its temperature and frequency dependent dielectric properties are investigated for a wide temperature (80-350 K) and frequency (1 kHz - 1 MHZ) ranges. The prepared compounds assume monoclinic $P2_1/n$ space group with estimated lattice parameters a=5.333 Å, b=5.565 Å, c=7.582 Å, α=90.0°, β=89.99° and γ=90°. Reasonably high value of dielectric permittivity around ambient temperature, and in the kHz frequency regime associated with relatively weak temperature sensitivity was noted. A correlation of frequency dispersion of dielectric constant with magnetic ordering was found. The observed broad and asymmetric dielectric relaxation peak in the electric modulus spectra deviates considerably from the ideal Debye type dielectric relaxation due to the influence of inhomogeneity and disorder. The high permittivity is attributable to the hopping polarization contribution of two dissimilar cations 'Co' and 'Mn' in the 'B'-sites of the mixed perovskite Eu_2CoMnO_6. The influence of the anti-site disorder was also detected in the Raman active modes detected around 498, 628, and 1250 cm^{-1}.

i) Transport properties

i0001

Quantum Transport Behavior of Hydrogenated Borophene

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Two-dimensional (2D) materials beyond graphene have gathered a large interest owing to reduced carbon footprint. Boron being the nearest neighbor of carbon has been explored for its 2D forms, where 2D boron nanosheet (borophene) has been experimentally grown on silver surface. Doping or functionalizing nanosheets adds exciting new properties to the existing known materials. Based on density functional and boltzmann theory, we report a comprehensive first-principles study of structural, electronic, and transport properties of β_{12} borophene in its pristine and hydrogen doped forms. We find that the dirac point (between Γ and X k-points) is well retained after doping the hydrogen atom into the β_{12} lattice site. However the increased metallicity due to additional electronic bands can also be explored for charge density wave formations. Regarding transport behavior, we find that hydrogen doping significantly enhance transport properties, with zigzag being the preferred direction at room temperature. Our work suggests that doping and/or functionalization can be used as an important parameter to tune the transport properties of boron nanosheets.

i0003

Polaronic and Magneto-Transport Properties Of Phase-Separated Sm(Ca,Sr)-Based Manganite Compound

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In this work, we have investigated the electronic and magnetic transport properties of half-doped single crystalline $Sm_{0.5}Ca_{0.25}Sr_{0.25}MnO_3$ manganite compound in detail. The compound exhibits a robust charge-ordered-insulating phase, which is destabilized upon application of a 30 kOe magnetic field. It also shows an ultra-sharp meta-magnetic-type transition due to the presence of quenched disorder and kinetically arrested metastable phases in the system. As a result, a metallic phase is permanently settled down with a huge value of magnetoresistance (MR) of the order of 10^{14}% at T = 25 K over a magnetic field sweep of 90 kOe. With this recorded value of MR, the compound can be utilized in magnetic data storage industries. The high-temperature semiconducting and low-temperature field-induced metallic states can be well-explained with the polaronic transport mechanisms such as the small polaron hopping model and various interaction-conduction mechanisms respectively.

i0004

Probing the Structural, Electronic, and transport properties of $Cs_2NaAmCl_6$ through DFT Simulation Methods

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We provide a comprehensive picture of the structural and magneto-electronic features of the $Cs_2NaAmCl_6$ halide double perovskite employing computations from density functional theory. The well-known generalized gradient approximation is implemented to evaluate the exchange-correlation potential. The alloy is ascertained to be stable in a cubic structure with Fm-3m symmetry by structural optimization. The electron occupancy in the f-orbitals of Am impacts the total electronic and magnetic properties of alloys. The spin-polarized band structure and density of states reveal that $Cs_2NaAmCl_6$ has a half-metallic nature with a broad bandgap in the spin-down state. The magnetic moment is observed to be 6 μB, with the Am-atom bearing the majority of the contribution. The half-metallic nature of $Cs_2NaAmCl_6$ with a large magnetic moment substantially facilitates its use in a spintronic field. Additionally, the transport properties of the proposed compound $Cs_2NaAmCl_6$ have been computed.

i0005

Origin of Low Temperature Resistivity Anomaly in Ti_2FeAl

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Here, we report the underlying mechanism for the origin of an anomaly in electrical resistivity in the low temperature regime of an inverse Heusler alloy, Ti_2FeAl. This alloy crystallizes in cubic structure (space group 216, $F\bar{4}3m$). The zero-field resistivity curve exhibits metallic behavior in high temperature regime and exhibits an upturn below 50 K with a pronounced minimum around 34 K. The nature of the observed upturn is robust under the applied magnetic fields. Interestingly, the temperature at which minimum is observed shifts towards lower temperatures on increasing magnetic field strength. Detailed analysis of the resistivity data reveals that at zero field, the combination of electron-electron interactions and Kondo effect results in the observed anomaly. Further, on application of magnetic field, the resistivity upturn is dominated by the electron-electron interactions.

i0006

Multiple Manifestations of Negative Partial Density of States

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Recently, it has been observed that in mesoscopic systems certain members of density of states (DOS) hierarchy like local partial DOS (ρ_{lpd}), partial DOS (ρ_{pd}), injectivity (ρ_i), emissivity (ρ_e), etc. can become negative wherein electrons move

back in time. This may have implications for the thermodynamic properties of these mesoscopic systems. In these negative local partial states, electrons may behave akin to positrons, resulting in practical the possibility of electron-electron interaction. The objective of this research is to reveal some manifestations, employing rigorous calculations utilizing two different approaches: a continuum model and a discrete or tight binding model. It has been demonstrated that negative local partial states are correlated with Fano-resonance featuring a π phase drop.

i0007

DFT Calculations on the Structural, Mechanical, Electro-magnetic and Transport Properties of Half-metallic $CsPuO_3$ alloy

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In this piece of work, we have scrutinized the structural, mechanical, electro-magnetic and thermoelectric properties of simple oxide-based perovskite CsUO3 within the framework of density functional theory. The structural stability and mechanical behaviour are defined by the optimization of total energy and calculations of elastic constants respectively. The band profile and density of states displays the half-metallic nature of the material which is further confirmed by integer value of magnetic moment. Finally, the different thermoelectric parameters like Seebeck, electrical conductivity, thermal conductivity and power factor are computed, which reflects the decent values of these parameters, addressing this material capable of being used for a green energy generation.

i0008

Synergistic Exploration of Structural, Electronic, Magnetic, and Thermoelectric Properties of $BaMn_4As_{12}$

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The $BaMn_4As_{12}$-filled Skutterduite material was analyzed using highly precise spin-polarized density functional theory (DFT). The analysis focused on its fundamental properties, including structural, electronic, and magnetic aspects. The material was found to have a cubic geometry with space symmetry Im3 (204), and the lattice constant agreed well with experimental results from similar materials. The band structure and density of states analysis revealed a metallic band character with the spin-up states exhibiting metallic behavior and the spin-down states showing metallic behavior. The material's spin magnetic moment was determined to be 5.11 μB, indicating its potential application in electrodes and spintronic-based devices. The thermoelectric response of the $BaMn_4As_{12}$ functional material makes it a promising candidate for waste heat recovery systems. The carefully studied ground state properties of $BaMn_4As_{12}$ offer valuable insights that could aid in the experimental synthesis of this material for use in future energy harvesting technologies and spintronic applications.

i0009

First-Principles Investigations of Structural, Electronic, and Thermoelectric Properties of Co-Based Semiconductor Half-Heusler Alloy

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With the help of density functional theory here, we have to analyse the structural, electromechanical and thermoelectric properties of half Heusler CoHfAs alloy. The structural result reveals non-magnetic phase is the most stable phase with optimized lattice parameters 5.83 Á, CoHfAs exhibit semiconducting behaviour in both spin channels with gaps of 1.175 eV and 1.375 eV in Generalized Gradient Approximation and modified Becke-Johnson potentials respectively. The mechanical properties of this alloy reveal its ductile nature. The transport coefficients are obtained by using Boltzmann theory. The overall results suggest that these materials can have applications in thermoelectric domains.

i0010

Emergence of A Hidden Topological Insulator Phase in Hybrid Halide Perovskites: A Novel Paradigm through Tip-Induced Electric Field

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We report the emergence of a hidden topological insulator phase in hybrid halide perovskites under the influence of a high tunneling electric field generated by bringing a scanning tunneling microscope (STM) tip to the close proximity of the sample. As witnessed from scanning tunneling spectroscopy (STS), the low-temperature orthorhombic phase of the compounds in its equilibrium behaves like a normal insulator with a bulk bandgap, that is, when the material was probed with a tip placed far away. When the set current vis-à-vis the tunneling electric field was increased with an approach of the tip, a Stark-effect-induced shift of the bands towards the Fermi level (E_F) was witnessed with a closure of the transport gap. At a (high) critical set current, the material turned into a 3D topological insulator with gapless surface states and a Dirac point below the E_F.

i0011

Thermoelectric Properties of KMgAs Half Heusler Compound: A DFT Study

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In the present study, a systematic investigation of structural, electronic and transport properties of KMgAs half-Heusler has been conducted using the FP-LAPW method investigated with DFT. The correlation effect is implemented with PBE-GGA, mBJ and mBJ+SOC as exchange potential. The electronic band plot reports the presence of an indirect energy band gap equal to 2.68 eV. The results demonstrate that our studied compound depicts a semiconductor with a p-type nature. Transport properties of the studied compound were estimated using semi-conventional Boltzmann theory under a constant relaxation time assumption at various temperatures, chemical potentials, and carrier concentrations.

i0012

Ab-initio Study of 2H-CrS_2 Monolayer for Thermoelectric Applications

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The present manuscript deals with the calculation of structural, electronic and thermoelectric properties of 2H-CrS_2 monolayer by employing ab-initio calculations in combination with the Boltzmann transport theory. Structural stability of this monolayer has obtained by drawing the phonon dispersion curve. Verification of semiconducting nature of monolayer is confirmed by getting the electronic bandgap of value 0.97 eV. Further, the thermoelectric properties such as large power factor, low lattice thermal conductivity and higher value of ZT = 0.62/0.56 for p-/n-type doping at temperature 300 K are obtained. This study suggests that the p-type 2H-CrS_2 monolayer can be used in thermoelectric devices.

i0013

Stokes-Einstein Breakdown and Dynamical Heterogeneity in Deep Eutectic Solvents

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In this study, we explore the relationship between the breakdown of the Stokes-Einstein (SE) relationship and dynamical heterogeneity in deep eutectic solvents (DESs). These DESs are known for their strong dynamical heterogeneity due to extensive hydrogen bond interactions. Using quasielastic neutron scattering measurements, we investigate the glassy dynamics of acetamide-based DESs with lithium salts. Our results reveal a decoupling between jump diffusion and viscosity, indicating a significant breakdown of the SE relationship, characterized by a fractional Stokes-Einstein (FSE) equation. Surprisingly, the strength of SE breakdown is found to be inconsistent with the degree of dynamical heterogeneity in this DES series. This work provides the first experimental evidence of contrasting features between dynamical heterogeneity and the breakdown of the SE relationship, challenging current understandings of their correlation.

i0014

Electronic Transport of $Zn_{0.2}Co_{0.8}Fe_2O_4$-Poly (vinylidene fluoride) Flexible Film With Wavelengths

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Multiferroic magnetoelectric materials have gained immense research interest because of their diversified and potential applications like memory device, sensor, energy harvester etc. We have fabricated Zn0.2Co0.8Fe2O4- poly (vinylidene fluoride) flexible nanocomposite film through low temperature pyrophoric reaction process next off solution casting method. Surface characterization has been carried out by SEM micrograph from. We have observed the variation of impedance with frequency of red and green laser light sources. It has been noticed that change of impedance is lower at the higher frequency region because of not getting sufficient time for polarization of charge carriers. At a frequency of 500 Hz, it has been observed that decrease of impedance is more (~2%) for green laser than red laser (~0.94%) at a intensity of 0.6 mW/cm2. The attempted research work yields indication about the effect of laser light on transport properties of the prepared nanocomposite flexible film.

i0015

Band Structure and Thermoelectric Properties of Topological Insulator LiAuSe by First-Principles Study

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The objective of this investigation is to analyze the structural, electronic, and thermoelectric transport characteristics of the LiAuSe compound, which is classified as a topological insulator. This study has been achieved by employing first-principles calculations and made use of the WIEN2k code, which employed the FPLAPW (Full Potential Linearized Augmented Plane Wave) method. The quantitative value of the negative band inversion provides us with valuable information regarding the existence of topologically nontrivial band features of the studied compound. The calculation of elastic constants reveals that LiAuSe exhibits excellent elastic and thermodynamic stability. Furthermore, the semi-classical Boltzmann transport equations were employed, which use constant relaxation time approximation. The Seebeck coefficient and power factor were measured to be 178.76μV/K and 3.95×10^{11} W/msK^2 respectively. At 1200 K, the figure of merit (ZT) is calculated to be 0.37, suggesting that LiAuSe can be efficient as a thermoelectric material suitable for high-thermal applications.

i0017

Pauli Blocking Effect on Chiral Electron-Phonon Relaxation in Bilayer Graphene; A Numerical Study

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Deformation potential chiral electron-phonon relaxation rate is calculated numerically for acoustic, optical and surface optic polar phonon modes for suspended and substrated Bilayer Graphene (BLG). The calculations have performed using Boltzmann transport equation with in relaxation time approximation considering the Pauli Blocking (PB) factor, which inhibits electronic transitions to the final filled transition states, particularly at higher temperatures. It is found that the relaxation rate in BLG is higher (one order about) than Monolayer graphene (MLG) for acoustic phonons and for optic phonons the relaxation rate in BLG is lower (one order about) than MLG. These trends in general are in conformity with the earlier reported studies. The scattering due to surface optic polar phonon mode for BLG placed on a substrate also has a relaxation rate enhanced by an order of magnitude as compared to MLG, and it dominates over both acoustic and optic modes. The sum of the relaxation rates due to all these three modes is found almost equal to the surface polar optic phonon relaxation rate.

i0018

The ARPES, Magnetotransport and Thermoelectric Properties of $Bi_{1.9}Gd_{0.1}Se_3$ Single Crystal

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In this present study, we have investigated the Angle Resolve Photo-emission spectra (ARPES) and Magneto-Transport study of $Bi_{2-x}Gd_xSe_3$ (x= 0.1) shiny plate like single crystal grown along c axis (confirmed by XRD study) prepared by modified bridgeman method. The resistivity data shows metallic nature throughout the temperature range (100K<T<300K) however at low temperature (<100K) the crystal shows a upturn behavior in resistivity known as Kondo effect which may be due to the gap opening at dirac point, further confirmed from ARPES. The nature of hall data and ARPES (the fermi level lies in the conduction band) confirm the n type majority carriers participated in the transport. The prepared crystal shows ~80% unsaturated linear MR value upto 8T and at low temperature and high magnetic field. To analyze the thermoelectric properties, we have conducted Seebeck measurement which gives a value of seebeck coefficient ~ -191 μV/K and a power factor ~ 1.3 mW/K^{2}m at room temperature which made the prepared sample efficient for thermoelectric applications

i0019

Role of Disorder in the Magnetotransport Property of WTe2- a type II Weyl Semimetal

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In this work, two different synthesis methods, Te-flux and the chemical vapor transport methods were adopted for the preparation of WTe_2 single crystals. XRD and EDX confirmed the pure phase of the as prepared single crystals. Metallic nature of the samples has been confirmed by the resistance vs. temperature graph. The estimated RRR value has been found decreased in the compound synthesized by the chemical vapor transport method. Magnetoresistance has been measured as a function of magnetic field at 50K and 100K up to ±7T for both the compounds. The maximum value of magnetoresistance in sample prepared by flux-method was as high as 270% at 50 K, while it is much lower in case of chemical vapor transport method (~ 23%). Disorder appears to be a key factor for deriving the magnetoresistance in this system.

i0020

Electrical transport properties of chromium orthovanadate from first principles simulations

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$CrVO_4$ displays strong spin-orbital coupling without relativistic interaction. Coupled Hamiltonian in such a system allows a sudden decrease in the electrical resistance upon application of external magnetic fields, a phenomenon known as colossal magnetoresistance (CMR)[1]. Here, we understand various contributions of orbital states near the Fermi level and find the role of such states in deciding the electrical resistivity and Seebeck coefficient for a wide range of temperatures. The results are comparable with earlier measurements below the thermal activation temperature of electrons. Our study helps us understand the electrical transport properties from the electronic structure of $CrVO_4$ and further motivates research to explore CMR.

i0021

INFLUENCE OF SINTERING TEMPERATURE ON VARIOUS PROPERTIES OF DOPED MANGENITE

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In the present communication, the structural, microstructural, and transport properties of sol-gel-grown nanostructured doped manganite $La_{0.5}Nd_{0.2}Ca_{0.3}MnO_3$ (LNCMO) were sintered at different temperatures (viz., 1000, 1100, and 1200°C). The Structural characterization was studied by X-ray diffraction (XRD). TEM was used to examine particle size and shape in order to better understand the microstructural characteristics. Transport properties result in modifications in the metal-insulator transition temperature (Tp), which gets reduced for higher sintered samples. The alternation in properties can be explained using grain morphology and the presence of oxygen vacancies at the grain boundary region.

i0022

Investigations on Transport Properties of Phase-Rich Charge-Ordered Manganite-Based n-n Junctions

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In the present communication, $CdO/La_{0.3}Ca_{0.7}MnO_3/Al_2O_3$ (CdO/LCMO/AlO) n-n junction based heterostructures, with various thicknesses of LCMO layer, were successfully fabricated using chemical solution deposition (CSD) method. X–ray diffraction (XRD) measurement confirms the presence of LCMO and CdO phases only without any other unwanted phases and validates the polycrystalline growth of CdO and LCMO over the polycrystalline Al_2O_3 substrate. The microstructural study, carried out by performing atomic force microscopy (AFM), shows the enhanced grain size and reduced rms surface roughness with an increase in film thickness. To understand the charge transport mechanisms across CdO/LCMO n-n junction and to study the intriguing phase of LCMO such as charge-ordered insulator, the temperature dependent resistivity measurement was performed in temperature range of 150K to 310K where the results show the Mott-type insulator behavior throughout the temperature range studied. The electrically insulating state of all the heterostructures have been studied using Mott type variable range hopping (VRH) mechanism. Observed charge-ordered insulator transition T_{CO} and anti-ferromagnetic insulator transition T_N have been discussed in detail with its dependence on temperature and manganite layer thickness. On the basis of Mott type VRH mechanism, interesting parameters such as activation energy E_a and density of states near fermi level $N(E_f)$ have been estimated and their dependence on temperature and thickness of manganite layer have been understood in detail for the phase-rich manganite based $CdO/LCMO/Al_2O_3$ heterostructures**.**

i0023

Anomalous Hall Effect in Semimetallic MnPtGa Single Crystal

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Anomalous Hall effect (AHE) is an interesting phenomenon observed not only in the magnetic system but also in non-magnetic compounds. Here we report the observation of a large anomalous Hall conductivity (AHC) in the spin-canted state of a magnetic single crystal MnPtGa crystallized in a centrosymmetric hexagonal structure (sp. gr. *P6₃/mmc*). MnPtGa orders ferromagnetically at T_C=250 K, below which a large magnetocrystalline anisotropy is observed, with the [0001]-axis being the easy axis of magnetization. For the field applied in the [0001] crystallographic direction, AHC of MnPtGa exhibits a nonmonotonic behavior and becomes negative below 115 K with the largest value of $-500\ \Omega^{-1}cm^{-1}$ that remains nearly constant below 20 K. Our observation suggests the intrinsic origin of AHE in MnPtGa.

i0024

Impedance Spectroscopy Analysis of Cr and Ni-doped $CaBaCo_4O_7$

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Complex impedance analysis is a technique which allows us to correlate electrical and microstructural properties. We have presented here the impedance analysis of $CaBaCo_4O_7$, $CaBaCo_{3.96}Cr_{0.04}O_7$ and $CaBaCo_{3.96}Ni_{0.04}O_7$. The analysis confirmed that the charge conduction occurs via nearest neighbour hopping in the low-*T* region. In the high-*T* region, conduction occurs via quantum tunneling of small polarons over a short range. Existence of non-Debye type relaxation mechanism within the materials also verified.

i0026

Magnetotransport In The $ZrAs_2$ Single Crystal

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The Single crystals of $ZrAs_2$ which crystallizes in the orthorhombic structure with the nonsymmorphic space has been grown by the flux method. We report the magnetotransport and quantum oscillation studies on this single crystal. The temperature dependent resistivity $\rho(T)$ shows a metallic behaviour in zero field, whereas there is a metal-to-insulator transition in presence of high magnetic field. Large magnetoresistance (about 1010% for $I \parallel [010]$, $B \parallel [105]$) with quadratic field dependence is observed without any sign of saturation up to the 14 T magnetic field. The carrier concentration is estimated from the field dependent Hall resistivity, and it is found that the charge carriers are nearly compensated which results in such large magnetoresistance. Shubnikov-de Haas (SdH) and de Haas-van Alphen (dHvA) oscillations have been observed at low temperature and high magnetic field.

i0027

Accelerating Discovery of Vacancy Ordered 18-Valence Electron Half-Heusler Compounds: A Synergistic Approach of Machine Learning and Density Functional Theory

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Abstract. In this study we attempted to model vacancy ordered half Heusler compounds with 18 valence electron count (VHH) derived from 19 VEC compounds such as TiNiSb such that the compositions will be $Ti_{0.75}NiSb$, $Zr_{0.75}NiSb$ and $Hf_{0.75}NiSb$ with semiconducting behavior. The main motivation is that such a vacancy ordered phase not only introduce semi conductivity but also it will disrupt the phonon conducting path in HH alloys and thus reduce the thermal conductivity and as a consequence enhance the thermoelectric figure of merit. In order to predict the formation energy (ΔH_f) from composition and crystal structure we have used 4684 compounds for their ΔH_f values are available in the material project database and trained a machine learning model with R^2 value of 0.943. Using this trained model, we have predicted the ΔH_f of a list of VHH. From the predicted database of VHH we have selected $Zr_{0.75}NiSb$ and $Hf_{0.75}NiSb$ to validate the machine learning prediction using accurate DFT calculation. The calculated ΔH_f for these two compounds from DFT calculation are found to be comparable with our ML prediction. The calculated electronic and lattice dynamics properties show that these materials are narrow band gap semiconductors and are dynamically stable as their all-phonon dispersion curves are having positive frequencies. The calculated Seebeck coefficient, electrical conductivity as well as thermal conductivity, power factor and thermoelectric figure of merit are analyzed.

i0028

Electrical transport in Li_2SO_4-Li_2O-P_2O_5-B_2O_3 Glassy Ionic system

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The structural and electrical transport in a glassy system of Li_2SO_4-Li_2O-P_2O_5-B_2O_3 is reported in the present investigation. X-ray diffraction (XRD) and differential scanning calorimetry (DSC) confirm the samples are amorphous and glassy in nature. The ionic conductivity exhibits an abnormal rise, diverging from Arrhenius behaviour, as a result of such structural relaxation at the glass transition temperature. It has also been discovered that the addition of B_2O_3 increases ionic conductivity.

i0029

Synthesis and Magneto-Transport Study of Kagome Metal Ni3In2S2

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The kagome-lattice crystal has several intriguing properties, such as frustrated magnetism, topological state, superconductivity, charge order and correlated phenomena. Here we report the synthesis and characterisation of the Kagome metal $Ni_3In_2S_2$ and study the transport properties of the Kagome metal. The crystal has a trigonal crystal structure with space group R-3m (No.-166). The transport measurement shows no magnetic phase transition with the temperature range of 50k to room temperature. $Ni_3In_2S_2$ has the classical origin of MR and also shows angle-dependent anisotropy in longitudinal resistance.

i0030

Structural, Electronic, and Electron Transport Property of Nickel-doped Porphyrin Two-Terminal Device with Graphene Electrodes

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Porphyrin, which is crucial to many biological processes, has attracted much attention as a molecular device for optoelectronic application. This study focuses on Nickel doped (Ni-doped) porphyrin-based single-molecule attached to graphene electrodes forming a two-terminal device molecular junction. The structural and electronic properties of Ni-porphyrin are studied by calculating the HOMO-LUMO gap, chemical hardness, binding energy of the metal, etc. We have further investigated the electron transport properties of Ni-doped porphyrin utilizing the non-equilibrium Green's function (NEGF) approach and density functional theory (DFT) and discussed the transmission coefficient and the current-voltage characteristics of a Ni-porphyrin molecule connected to two armchair graphene electrodes by triple-bonded carbon atoms as an anchoring group. We

obtained the I-V curve of the two-terminal system by applying a bias to the molecular junction in steps of 0.2V ranging from -1.0V to +1.0V while studying the evolution of the transmission spectrum on changing bias. Along with a rise in current, an NDR (negative differential resistance) behavior is observed when applying increasing positive and negative biases.

i0031

Harmonically confined particle in a viscoelastic suspension

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We study the self-propulsion of an inertial active Ornstein-Uhlenbeck particle confined in a two dimensional harmonic well and suspended in a viscoelastic suspension. From the exact solution of the dynamics, we have established a phase diagram separating the oscillatory and non-oscillatory phases of the motion. By exploring the diffusive behaviour of the particle, we observed that the mean square displacement (MSD) shows ballistic feature of motion in the initial time regimes, whereas it is non-diffusive in the time asymptotic limit or at steady state. Further, by the interplay of different time scales involved in the dynamics, the steady state MSD gets suppressed with increase in the persistent duration of activity and gets enhanced with increase in persistent duration of elastic dissipation in the medium.

i0032

Electrical Charge Conduction Mechanism in Sm^{3+} and Yb^{3+} Doped La_2NiMnO_6 Double Perovskites at Low Temperature Regime

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The temperature dependent magnetic and electrical current-voltage (I-V) characteristics of Sm and Yb doped La2NiMnO6 (LNMO) samples have been investigated. The magnetization curve revealed the ferromagnetic behavior of Sm and Yb doped samples. The electrical conductivity is calculated from I-V characteristics demonstrated their semiconducting nature and measurements confirmed the types of conduction mechanisms (in the temperature range 10–300 K) for Sm and Yb doped samples. The conductivity curves are dominated by Poole-Frenkle (thermally activated band conduction) as well as Mott's variable range hopping (VRH) conduction mechanism at higher temperature regime, whereas Mott's variable range hopping (VRH) conduction is dominated at lower temperature range. The variation in conductivity curves of Sm and Yb doped LNMO samples is found near their magnetic transitions, suggesting a correlation between electrical and magnetic properties.

i0033

Thermophysical properties of molten salt LiF-NaF-KF for application as a coolant in nuclear reactor: Molecular dynamics simulation

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Molten salts have important roles in nuclear technology and other applications. Examples are like use as coolant and fuel in nuclear reactors and as solvent for pyrometallurgical recycling process. Work has been carried out to estimate various important transport properties of molten salt LiF-NaF-KF for a range of composition and temperature applying extensive Molecular Dynamics simulations here in this paper. We are reporting estimated values of Velocity Auto Correlation Function (VACF), Onsager coefficients, MS diffusivity, entropy etc. for the above mentioned salt. Diffusion coefficient for Li-Li ion pair is found to be the highest. Similar is the value for F-F ion pairs. Backscattering effect for different cation-anion pairs are significant, indicating no movement of the ions whereas it is not so for cation-cation or anion-anion pairs. We have observed negative MS diffusivity for cation-cation ion-pairs only and not in anion-cation ion pairs. But the positive entropy for these negative MS diffusivities are assured to confirm the second law of thermodynamics.

i0034

Transport Measurement in HgTe Single Crystals

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The search for symmetry protected topological states in quantum materials has attracted a lot of interest in the field of condensed matter physics. Dirac, Weyl, and nodal line semimetals are crystalline solids whose low energy excitations resemble the Dirac and Weyl fermions that were predicted in high energy physics. In crystalline systems with additional symmetry protection, can lead to topological protection of the surface states and interesting phenomenon like large unsaturated magnetoresistance, quantum anomalous Hall effect, and non-trivial Berry phase in quantum oscillations. Hence studies on these systems enables us to understand underlying physics and prepare the groundwork for further applications. HgTe is a versatile topological material and has enabled the realization of a variety of topological states, including two- and three-dimensional topological insulators and topological semimetals. Topological Insulators are new states of matter possessing a topological order induced by a strong spin-orbit. One of the hallmarks of this topological order is the appearance of robust

surface states, owing to which quantum spin Hall (QSH) effect was first reported in HgTe quantum wells. We have grown the HgTe single crystal which is a topological insulator and transport measurements show a semiconductor to semimetal transition indicating the presence of conducting surface states leads it to transition to semimetal.

i0035

Structural and Transport Behavior in Bulk and Films of $Pr_{0.6}Sr_{0.4}MnO_3$: The Role of Lattice Strain

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Here, we investigate the structural and transport properties of both bulk and thin films of $Pr_{0.6}Sr_{0.4}MnO_3$. Epitaxial films, with thicknesses of 10nm and 20nm have been grown on $SrTiO_3$ (100) substrate using pulsed laser deposition (PLD) method. Structural investigation of $Pr_{0.6}Sr_{0.4}MnO_3$ has been done using x-ray diffraction (XRD) and Rietveld analysis. $Pr_{0.6}Sr_{0.4}MnO_3$ crystallizes in orthorhombic crystallographic phase with *Pbnm* space group. Atomic Force Microscopy (AFM) data reveals that the thin films exhibit good surface morphology. Electrical resistivity data of bulk $Pr_{0.6}Sr_{0.4}MnO_3$ exhibits a metal insulator transition (MIT) at $T_{MIT} \sim 244$ K, which follows power law equation. In contrast to the bulk material, the resistivity data for the thin films $Pr_{0.6}Sr_{0.4}MnO_3/SrTiO_3$ (10nm and 20nm) shows an insulating behaviour across the measured temperature range, where the resistivity increases with decreasing film thickness. While the charge conduction mechanism in films is found to follow the Mott's 2D Variable-Rane-Hopping (VRH) model, this strain induced tuning of conduction remains quite intriguing.

i0036

The Structural and Transport Properties of $CaMnO_3$ Bulk and Thin film

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We have studied the structural and electrical transport properties of CaMnO3 perovskite. Epitaxial thin film of CaMnO3 has been prepared on LaAlO3 (100) substrate using the pulsed laser deposition (PLD) technique. Structural investigation has been done using x-ray powder diffractiopn and Rietveld analysis. CaMnO3 crystallizes in orthorhombic crystal structure with Pnma space group. The resistivity of bulk CaMnO3 shows insulating behaviour, at low temperature which follows with Motts 2D variable range hopping (VRH) model. Atomic Force Microscope (AFM) has signified the good quality of the films.

i0038

Dwelling In Conductivity and dielectric response in Mixed Alkali Composition (NaxLi(1-x))4NbP3O12 Glasses

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A new mixed alkali Niobium based NASICON phosphate glasses with a composition $(Na_xLi_{(1-x)})_4NbP_3O_{12}$ were prepared and characterized by XRD, DSC, FTIR as well as Impedance Analyzer. XRD conforms amorphous nature and FTIR various phosphate vibrations. Thermal study reviled the mixed alkali effect in the glass transition temperature. Impedance, ac conductivity and dielectric spectroscopy are employed in the frequency range 10Hz–1MHz at different temperatures to examine the electrical data. The frequency dependence of conductivity has been analyzed using Almond–West expression and the dc conductivity and the hopping frequency were obtained. The minimum in dc conductivity and hopping frequency are obtained at the mixed alkali composition, where their activation energy are the same. A few interesting aspects of scaling of temperature and composition dependence of ac conductivity. electric modulus and Dixon scaling are also reported in the presence of mixed alkali. is the standard font and layout for the individual paragraphs.

i0039

Transport properties of XZnN (X= Li/Na) Half Heusler: A DFT Insight

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Abstract. In the present study, CONSIDERING first-principles calculations and the Boltzmann transport theory, we have analyzed the structural, mechanical, vibrational, optical, and thermoelectric properties of the XZnN (X= Li/Na) half-Heuslers (HH). The exchange-correlation effect is considered using the generalized gradient approximation (PBE-GGA), TB-mBJ. According to the TB-mBJ technique, the investigated XZnN (X= Li/Na) HHs possess bandgap 1.92 eV, 1.71 eV respectively. To calculate elasticity coefficients, such as Young's modulus(E), shear modulus (G), bulk modulus (B), and mechanical properties like Pugh's ratio (B/G), anisotropic factor (A), etc., three elastic coefficients C_{11}, C_{12} and C_{44} are computed. are used. The transport properties for the XZnN (X= Li/Na) are determined. At a temperature of 1200K, figure of merit (ZT) is 0.88, and 0.83 for XZnN (X= Li/Na) suggesting these may be employed in thermoelectric generators.

j) Semiconductor and spintronics

j0003

Defect Induced Magnetism In Hybrid Perovskite: A Combined First-principle And Experimental Study

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Organic inorganic hybrid perovskite is an excellent photovoltaic material due to its exceptional optoelectronics properties. Defect induced ferromagnetism in direct band gap semiconductor opened up a new concept in basic science research. In this present work, we employed first principle calculation to understand the defect induced magnetic property in hybrid perovskite material. The lead vacancy and iodine vacancy can induce significant amount of magnetic moment in hybrid perovskite systems. P-d exchange interaction in the vicinity of defects generate the magnetic moment. In the later part, we have shown that a significant amount of magnetic moment aroused in hybrid perovskite material due to lattice defect. Squid measurement confirms ferromagnetic ordering in defect induced hybrid perovskite. Therefore, the theoretical and experimental; observation suggest that significant amount of defect can induce ferromagnetism in these hybrid perovskite material which will be suitable for future spintronics applications.

j0004

Structural, Morphological, And Photo Response Tuning Of Semiconducting $CuBi_xIn_{1-x}Se_2$ Microrod Flowers For Photodetector Application.

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Whilst $CuInSe_2$ and $CuInGaSe_2$ are extremely promising materials for solar cell application, the shrinkage of the bandgap is highly desirable for transparent/semitransparent optoelectronic applications. Such shrinking has been achieved by replacing In with Bi in this report, along with the current-voltage response for photodetector application. The $CuBi_xIn_{1-x}Se_2$ microrod flowers (x = 0, 0.4, 0.8) were synthesized by microwave synthesis by taking different Bi/In concentrations, which allows alteration in structural, morphological, and optical behaviors. The $CuInSe_2$ showed polycrystalline nature, while Bi incorporation led to the appearance of Bi_2Se_3 phase. The Raman vibrational bands shifted with change in Bi/In content, indicating the composition variation induced structural transformation inside the matrix. Morphological analysis showed the transition from micro rods to cluster microrod flowers with the introduction of bismuth. The optical absorption is enhanced with different Bi/In content due to the enhancement in the microrod size, forming a flower structure. This reduces the optical bandgap by increasing defects and disorders in the forbidden gap. The photocurrent response reduced from μA range to nA range with varying voltage and composition.

j0005

Probing the Spin Configuration of *d*-states in a Manganese-Doped Semiconductor through Spin-Polarized Scanning Tunneling Spectroscopy

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We probe the spin configuration of manganese's d-states, in doped semiconductor quantum dots (QDs) through spin-polarized scanning tunneling spectroscopy (SP-STS). We show that the two levels have opposing spin-states. Experimentally, we probed the density of states (DOS) of the undoped and manganese-doped ZnS QDs, which have a wide band gap so that the $^4T_1$ and $^6A_1$ energies lie within the gap, through a nonmagnetic and a spin-polarized tip. While a nonmagnetic tip could inject electrons to $^4T_1$ and withdraw electrons from the $^6A_1$ state as well, the DOS derived with a spin-polarized tip evidenced that the tip could "see" only one of the two energy levels, whose spin-state remained parallel to that of the tip. The intensity of DOS representing the $^4T_1$ and $^6A_1$ of manganese thereby depended on the mutual alignment of the magnetization vectors representing the tip and the d-states. We have inferred that the spin configuration of $^4T_1$ and $^6A_1$ states in a manganese-doped wide band gap semiconductor could be probed through SP-STS and is mutually antiparallel in nature; such results have been the rationale of the photoluminescence (PL) emission in such manganese-doped QDs to possess an exceptionally long lifetime (~ ms).

j0006

Longitudinal Spin Seebeck Effect On Single Crystal $Y_3Fe_5O_{12}$

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Abstract. As heat is omnipresent and can be used efficiently by converting heat into electrical energy using spin degree of freedom. This can be achieved by spin Seebeck effect, which refers generation of spin current caused by a temperature gradient in a magnetic material. The spin current can be electrically detected on the deposited metallic film via inverse spin Hall effect. Here we report single crystal growth of $Y_3Fe_5O_{12}$ (YIG) using optical floating zone technique and its results, then longitudinal spin Seebeck effect (LSSE) measurements on indigenously developed LSSE measurement setup in Pt/ single crystal YIG system. The observed LSSE voltages (V_{ISHE}) have nice *V-H* loops at different temperature gradients.

j0007

Magnetic and Semiconducting Properties of Hydrothermally Synthesized CoS_2 Nanoparticles

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In this paper we report on the hydrothermal synthesis of CoS_2 nanoparticles and their magnetic as well as semiconducting properties. The characteristic properties of Schottky barrier diode were investigated using dc current voltage (I-V) measurement. The diode parameters including ideality factor and barrier height were calculated using Cheung and Cheung's method. DC Magnetization shows magnetic anomaly at 54 K which is irreversible under ZFC-FC protocol. We have tried to established a relation between the magnetic spin and metal- semiconducting behavior of CoS_2 nanoparticles. The observation of intrinsic ferromagnetism along with the variation of magnetization with magnetic field and temperature exhibits the suitability for spin based electronic application.

j0008

Exploring Photonic Absorbance and Photoluminescence Properties of $BiFeO_3$, $NiFe_2O_4$, and $BiFeO_3$@$NiFe_2O_4$ Core-Shell Nanocomposite Materials.

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In this study, $BiFeO_3$ (BFO), $NiFe_2O_4$ (NFO), and $BiFeO_3$@$NiFe_2O_4$(BFO@NFO) core-shell nanoparticles were successfully synthesized by sol-gel method. The structural characterization through Braggs reflection X-ray analysis confirmed the formation of rhombohedral BFO, cubic NFO, and BFO@NFO nanoparticles. By investigating the photonic absorption and photoluminescence properties of these nanocomposites, we observed a significant cross-band absorption between the core and shell materials. Consequently, the band gap energy of the nanocomposite was lowered, leading to reduced emission intensities in the photoluminescence spectrum. This decrease suggests improved segregation and transfer of photogenerated charge carriers at the BFO-NFO interface. Electromagnetic wave absorption enables practical applications in diverse fields, including stealth technology, radar-absorbent materials, medical imaging, and renewable energy harvesting, making it a fundamental aspect of modern technology.

j0009

Structural, Optical and Electrical properties of $Fe_{1.8}Co_{0.1}Ti_{0.1}O_3$ System

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$Fe_{1.8}Co_{0.1}Ti_{0.1}O_3$ oxide has been prepared using mechanical alloying of Fe_2O_3, CoO and TiO_2 powders, followed by subsequent heat treatment at 800° C in air and under vacuum. The X-ray Diffraction patterns and Raman spectra have validated single phase stabilization of rhombohedral structure. The current-voltage (I-V) measurement has shown Semi-conductive nature of this sample. The details of structural refinement parameters, optical and electrical properties of the samples have been presented in this work.

j0010

Giant Dielectric Constant and Magnetocaloric Effect in $EuTbCoMnO_6$ double perovskite

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The dielectric and magnetic behavior of double perovskite $EuTbCoMnO_6$ have been reported. X-ray diffraction confirms the presence of orthorhombic crystal structure of $EuTbCoMnO_6$ with space group Pnma. The dielectric measurement reveals the existence of strong dielectric relaxation with a giant dielectric constant near room temperature. Further, temperature-dependent magnetization confirms a second-order magnetic transition around 113 K. A maximum entropy change has been observed around ordering temperature, suggesting a magnetocaloric effect in the system.

j0011

Electrical Properties of Metamagnetic Eu_2CoMnO_6

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We report on the electrical and magnetic properties of polycrystalline Eu2CoMnO6. The X-ray absorption spectroscopy shows the mixed valance states of Co/Mn cations. The resistivity measurement shows the semiconducting nature of Eu2CoMnO6. Dielectric measurement shows a large dielectric constant at room temperature. The magnetization measurement shows that the

system has a strong metamagnetic state due to the coexistence of ferromagnetic (FM) and antiferromagnetic (AFM) ordering owing to the presence of antisite disorder and antiphase boundary.

j0012

Study of Spin Dynamics In Ferrimagnet Heterostructure

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Insulator garnets are now the most preferred candidates for spintronics applications due to their efficient magnetization dynamics. Recently, $Y_3Fe_5O_{12}$ (YIG) is studied extensively for quantum computation and magnon based spin current. In this context, we have studied the damping properties of pulsed laser deposited YIG and $Tm_3Fe_5O_{12}$ (TmIG) garnet films as well as their bilayers with Pt layer on the top. The enhanced damping value of the samples with Pt motivated us to study the spin pumping by FMR. Moreover, the angle dependent ISHE measurements shows maximum spin pumping voltage for YIG in the sample GGG (111)/TmIG(35 nm)/YIG(100 nm) /Pt(5 nm). This can be attributed to the high quality YIG layer with sharp interface with TmIG layer. The obtained results are relevant for a broad class of magnonic systems with overview of the spin transport.

j0013

Enhanced Optical Modulation of AC and DC Transport Property of $Zn_{0.3}Ni_{0.7}Fe_2O_4$ Heterostructure at Low Temperature

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We have investigated light dependent DC and AC transport properties of Si/ $Zn_{0.3}Ni_{0.7}Fe_2O_4$/CuPc/Au heterostructure at low temperature region. Under the illumination of red laser light (660 nm) photo-response has been observed at the interface of the heterostructure, which is enhanced at low temperature region. Like DC transport properties of the heterostructure, AC transport properties are also modulated under the illumination of light at low temperature region. All the impedances Z, Z' and Z'' are found to be strongly decreased at low temperature as compared to room temperature, due to enhanced photogeneration effect at low temperature region. Single resonance peak which is associated with the dielectric relaxation of the heterostructure is shifted towards the higher frequency region under illumination of light at low temperature region. Nyquist curves which are distorted semicircular indicates non-Debye type electrical relaxation process. Area of the Nyquist curves strongly decreases at low temperature suggesting higher photogeneration effect at the interface of the heterostructure.

j0014

Optical Tunability of Magneto-transport and Electrical Hysteresis in p-Si (100)/$La_{0.7}Sr_{0.3}MnO_3$/CuPc/Au Heterostructure Device: A Temperature Variation Study

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Abstract. Temperature dependent magnetic and photoresponse study of a hybrid organic-inorganic bilayer in the range of 300 K to 50 K has been carried out. There is a strong electrical hysteresis in our device. By further analysis of impedance spectroscopy data, we have confirmed that the electrical memory effect is arisen from charge storage at LSMO/CuPc interface and a strong interfacial dipole formation at that interface. The photogeneration in our device increases with the decrease in temperature. This effect may come from the temperature dependent shifting of energy band positions at the bilayer interface.

j0016

Impact of Post Annealing on Anode Buffer Layer in Inverted P3HT:PC61BM Bulk Heterojunction Solar Cell

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Present study explains, enhancement of efficiency in inverted organic photovoltaic (iOPVs) cell fabricated with synthesized electron transport layer ZnO/RGO nano composites, poly (3-hexylthiophene-2,5-diyl): [6,6]-phenyl-C61-butyric acid methyl ester and MoO_3 hole transport layer were utilized. In this study to explain the improve the device efficiency through post heat treatment. Synthesized materials were characterized by HRTEM and current voltage characteristics. We obtained 2.38 % efficiency after post heat treatment.

j0018

100 MeV Sulphur Ion Irradiation Effects on N-Channel MOSFETs at Different Biasing Conditions

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N-channel depletion MOSFETs were irradiated with 100 MeV Sulphur ions in the dose range of 100 krad to 100 Mrad at different gate biasing conditions (-4, 0, +4 V). The pre-irradiated and post-irradiated electrical characterizations were done at room temperature (300K). The different electrical parameters of MOSFET such as threshold voltage (V_{th}), density of interface trapped charges (ΔN_{it}), density of oxide trapped charges (ΔN_{ot}) and leakage current (I_L) were studied as a function of total dose. A considerable increase in ΔN_{it} and ΔN_{ot} and decrease in V_{th} was observed after ion irradiation. The results of all the irradiations at different gate biases were compared with each other and found that the degradation is more for the devices irradiated at positive gate voltage (+4V).

j0019
Optical and Photocatalytic Assessment of Visible Light Active Fe_2WO_6
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Abstract. The current study presents the optical absorbance, photoluminescence and photo-catalytic properties of Fe_2WO_6 and its efficacy to degrade the Methylene Blue (MB) dye in the visible light. The compound crystallized in orthorhombic structure with the pbcn space-group symmetry. The purity is determined by the FTIR spectrum. The compound demonstrated a band-gap of ~1.87 eV in the visible light region., which could be applied as a visible light active Luminescence and photo-catalyst. It is observed that the compound has effectively degraded the Methylene Blue under visible light within 40 Min with degradation up to 63 %.

j0021
Ferromagnetic Resonance Study on Quasi 2D Ferromagnet Fe_5GeTe_2
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Quasi-two-dimensional van der Waals materials, characterized by extensive ferromagnetic order, are now a key domain for advancing innovative spintronics and quantum devices in the future. Here, we examined the spin dynamic magnetization of polycrystalline Fe_5GeTe_2 using broadband ferromagnetic resonance (FMR) spectroscopy. FMR measurement analysis shows an effective magnetization of Fe_5GeTe_2 is 0.67 kOe which is consistent with prior VSM findings in literature.. Polycrystalline Fe_5GeTe_2 exhibits broad linewidth of 0.69 kOe which is comparable to soft 3D transition metal magnet. It is due to inhomogeneous line broadening and inherent Gilbert damping. Additionally, we developed designed microwave signal processing device using this material and evaluating its functionality as both a microwave band-reject filter and an adjustable phase shifter in the off-resonant region. The stop-band response can cover from 5 to 25 GHz with an applied magnetic field up to 7 kOe. High attenuation is -5 dB/ cm for Fe_5GeTe_2 based filter at 7 kOe applied magnetic field. Optimal differential phase shift studied for Fe_5GeTe_2 based phase shifter in high frequency region (18GHz) is approximately 10°/cm.

j0022
Magnetic and thermoelectric properties of TaFeSb based 2D Heusler phases
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TaFeSb has been studied for its excellent thermoelectric properties. To explore the novel phases, we have studied the 2D phases (Heuslerene) based on TaFeSb half Heusler alloy. The density functional theory-based calculations have been used to probe structural, electronic, magnetic and thermoelectric properties of these materials. Heuslerene phases with different stoichiometries (TaFeSb, Ta_2FeSb, $TaFe_2Sb$, $TaFeSb_2$) have were studied, the non-stoichiometric phases are found to be affecting the stability, magnetism and thermoelectric properties. In the end, spin Seebeck coefficient and spin-dependent Seebeck coefficients are reported.

j0024
Insights into Structural and Electro-Optical Properties of Lithium Tantalate ($LiTaO_3$) Ceramic: A Combined Experimental and DFT Analysis
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We've conducted an extensive investigation into the properties of $LiTaO_3$ ceramic, encompassing its structural, optical, electronic, and vibrational attributes. The X-ray diffraction (XRD) assessment of LiTaO3 demonstrated successful confirmation of a single crystal phase structure through Rietveld refinement-fitted XRD data within the triangular R3c space group. The optical assessment indicated a wide bandgap ceramic, exhibiting photoluminescence in the blue segment of the

visible spectrum. The optical energy bandgap was assessed using UV-Vis spectroscopy, with the electronic band gap calculated through Density Functional Theory closely approximating the experimental value. Upon illuminating the sample with λ_{exc}~325 nm, photoluminescence response was noted, emanating emission within the visible range. Notably, the determined band gap renders the material a promising candidate for photo-catalytic activities, particularly in overall water-splitting applications.

j0025

Study on Structural and Band Alignment Properties at the NiO/GaN Heterojunction Using Synchrotron Radiation Based Techniques

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Epitaxial layer of NiO has been deposited on GaN template using RF magnetron sputtering deposition technique. The crystalline quality and the epitaxial relationship have been investigated by X-ray diffraction at BL-13, Indus-2, Synchrotron source, using omega-2theta ($\omega/2\theta$) and phi (ϕ) scans in x-ray diffraction. The out-of-plane and in-plane epitaxial relationship for the NiO layer with respect to GaN is $[111]_{NiO} \parallel [0002]_{GaN}$ and $[11\bar{2}]_{NiO} \parallel [10\bar{1}0]_{GaN}$, respectively. The epitaxial NiO layer is found to have two domain structures oriented along the [111] direction with an in-plane rotation of 60° with respect to each other. Photoelectron spectroscopy measurements carried out at BL-10, Indus-2, have been used to determine the valence band offset and the band alignment at the NiO/GaN heterojunction (HJ). A type-II band alignment is observed at the HJ with valence and conduction band offset values of 1.1 ± 0.1 eV and 2.0 ± 0.1 eV, respectively. Since, NiO (Eg = ~ 4 eV) and GaN (Eg = ~ 3.2 eV) are wide band gap semiconductors, and a Type-II band alignment has been observed at their HJ, the experimentally determined values of band offsets can be used to design wide band gap optoelectronic devices based on NiO/GaN HJ.

j0026

Electrical Parameters and Series Resistance Analysis of Au/VO_2/P-InP/Pt Schottky Barrier Diode by Introducing A Vanadium Dioxide Interlayer.

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Abstract: In the present study, the electrical characterization of Schottky barrier diode (SBD), based on vanadium dioxide (VO_2) have been investigated at room temperature. The main electrical parameters of Au/VO_2/p-InP/Pt SBD has been determined from current-voltage (I-V) characteristics, using various methods at room temperature. The measured ideality factor (n), series resistance (Rs), and barrier height (Φ_b) of Au/VO_2/p-InP/Pt SBD are found to be 1.52, 680 Ω and 0. 92 eV respectively. The modified Norde method is also used to evaluate the Φ_b and R_S of the SBD and the corresponding values are 0.92 eV and 198 MΩ respectively. Moreover, Cheung's functions are used to extract the BH and Rs of the Au/VO_2/p-InP/Pt SBD respectively. The series resistance (Rs) is calculated by Cheung's functions and the corresponding values are 375 Ω and 375 Ω from the dV/d(lnI) versus I and H(I) versus I plots, respectively.

j0027

DFT Study of Structural, Electronic and Magnetic Properties of $Ga_{0.875}Cr_{0.125}P$

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The theoretical calculations of structural, electronic, and magnetic properties of $Ga_{0.875}Cr_{0.125}P$ Diluted Magnetic Semiconductor (DMS) in Zinc Blende phase (B3) have been performed using Density Functional Theory (DFT) as implemented in the Spanish Initiative for The Electronic Simulations with Thousands of Atoms (SIESTA) code with LDA+U (U=3) exchange-correlation (XC) potential. The study of spin polarized electronic band structures and magnetic properties represents induction of half metallic ferromagnetic behaviour in $Ga_{0.875}Cr_{0.125}P$ with 100% spin polarization. The hybridization of Cr-3d states with s and p states of Ga and P develops some local magnetic moment on non-magnetic Ga and P atoms.

j0029

Structural and morphological study of bulk and thin film Co_2MnSi/Si Full Heusler Alloy

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The recent development in spintronics has put half-metallic ferromagnetic materials at the centre of scientific research and applications owing to the theoretical existence of 100% spin polarization of the electron states at the Fermi level along with high Curie temperatures beyond room temperature. In this context, an arc furnace prepared Co_2MnSi (CMS) ingot is deposited

by electron beam on a Si (100) substrate. The prepared CMS ingot and deposited film is characterized from structural and Morphological points of view. The absence of foreign element and stoichiometric formation of CMS is determined by Energy-dispersive X-ray analysis (EDAX) which supports the purity and formation of CMS determined by X-ray diffraction (XRD) spectrum.

k) Magnetism and superconductivity

k0001

Crystal Structure and Thermodynamic Properties of RTaO4 (R = Ho and Gd)

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Here we report the structural and thermodynamic properties of orthotantalates HoTaO4 and GdTaO4, studied via X-ray diffraction and heat capacity measurements. Both, HoTaO4 and GdTaO4 crystallize in monoclinic structure, but in different space groups, P2/c (no. – 13) and I2/a (no. – 15). High temperature heat capacity is understood by the contribution of Debye and Einstein lattice terms. In the low temperature regime, both compounds show significant Schottky contribution. The magnetic field dependent heat capacity shows the variation in the position of anomaly with temperature, which appears due to the Zeeman splitting of electronic energy levels.

k0002

Unraveling the Combined Influence of Oxygen Vacancy and B-site Disorder on Exchange Bias in Magnetically Frustrated Poly-crystalline Compounds

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Perovskite systems have garnered significant attention for exploring emergent functionalities. By carefully controlling oxygen vacancies, we achieved a remarkable intrinsic giant exchange bias in $SrFe_{0.5}Co_{0.5}O_{3-\delta}$ (SFCO) with a substantial exchange bias field of 1.48 Tesla and a coercive field of 1.45 Tesla. Furthermore, we introduced B-site disorder by doping the system with 10% iridium (SFCI), resulting in a lower irreversible temperature and an enhanced exchange bias of 1.86 Tesla. Magnetic analysis revealed a notable enhancement in the exchange bias effect due to the presence of significant ionic mixtures. Our research aims to investigate the influence of oxygen deficiency and B-site disorder on exchange bias in oxide materials for potential
technological application.

k0003

On the Influence of A-site Cation in Controlling Structure and Magnetism of A2MnTiO6 (A = Ca, Sr, Ba)

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Double perovskite compounds, A_2MnTiO_6 (A = Ca, Sr, Ba) synthesized in ambient conditions by solid state reaction method have been studied for their structural and magnetic properties. Detailed analysis of X-ray diffraction data shows that these three compounds crystallize in three different structure types. Effect of A site radius and electronic configuration on the structural properties of double perovskites A_2MnTiO_6 (A = Ca, Sr, Ba) is clearly visible. With changing electronic configuration, Ca ($4s^2$) → Sr ($5s^2$) → Ba ($6s^2$), the structure of the compound changes from orthorhombic (Ca) → tetragonal (Sr) → hexagonal (Ba). Interesting magnetic properties have been observed in all the three compounds, especially for Ca, which exhibits negative magnetization.

k0004

Unusual Magnetic and Transport Properties of RFe2Al8 (R = La, Ce)

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Structural, magnetic, thermal and electrical transport measurements have been carried out on polycrystalline samples of RFe_2Al_8 (R = La, Ce) compounds and some interesting observations have been made. Both the compounds are stable in air and crystallize in an orthorhombic structure, space group Pbam. In the magnetic susceptibility measurements, the lanthanum compound exhibits a broad hump over the entire temperature range with maxima centered around 50 K, whereas the cerium compound exhibit features attributable to intermediate valence with a short-range magnetic order at ~3.9 K. Both compounds exhibit metallic behavior in the resistivity from room temperature till the lowest temperature of measurement, however, it has been observed that resistivity of La compound is higher than that of Ce compound at the lowest temperature, whereas it is other way round at the room temperature. Heat capacity measurements carried out for both the compounds rules out long range magnetic ordering, however, the $C_p(T)$ for La is higher than that of Ce around room temperature, implying higher contribution from phonons in La case. It is interesting to observe here that cerium compound exhibits intermediate valence under magnetic fields up to 2 Tesla, which was not observed earlier at this field. Details of these studies are presented and discussed in this work.

k0005

Structural and Magnetic Properties of V-Ti-Si Alloy Superconductors

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The structural and magnetic properties of the as-cast and annealed $V_{0.6-x}Si_xTi_{0.4}$ (x = 0, 0.05, 0.10, 0.15) alloy superconductors are reported here. It is found that addition of silicon to the V-Ti alloys results in eutectic precipitation of Ti_5Si_3-phase in the body centred cubic (bcc) β-V-Ti matrix. In the as-cast $V_{0.6-x}Si_xTi_{0.4}$ alloys, the superconducting transition temperature (T_C) changes non-monotonically with increasing silicon content whereas after annealing, it is about 7.7 K for all the alloys. On the other hand, the upper critical field decreases and the coherence length increases after annealing in the x = 0.10 alloy. The variations in the superconducting properties in the alloys are related to the solubility of 6 at.% Si in the $V_{0.60}Ti_{0.40}$ alloy and the vanadium enrichment in the β matrix due to the precipitation of Ti_5Si_3 phase.

k0006
Ambient Temperature Growth and Superconducting Properties of Ti-V Alloy Thin Films
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A study on the optimization of ambient temperature growth and superconducting properties of Ti-V alloy thin films grown on SiO_2-coated Si substrate is reported here. These films have been synthesized by co-sputtering of Ti and V targets, and films having different Ti concentrations were deposited to get the optimized critical temperature (T_C) of thin films close to the bulk value. The maximum T_C of 5.2 K has been obtained in the $Ti_{40}V_{60}$ composition, which is further increased to 6.2 K when a 10 nm thick Ti underlayer is added below the Ti-V film. GIXRD measurements confirm the formation of Ti-V alloys in the desired crystal structure. The upper critical field (H_{C2}) of the thin films has been estimated with the help of magnetotransport measurements. The utility of Ti-V alloy thin films in superconducting radiation detection applications is ascertained.

k0007
Magnetic And Magnetocaloric Properties Of Nanocrystalline Sample Of A Glassy Ferromagnetic Compound
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The modification of magnetic interactions due to the reduction of particle size has been explored in the case of nanocrystalline Gd0.5Sr0.5MnO3 compound. In contrast to the normal ferromagnetic or antiferromagnetic compounds, the studied nanoparticle exhibits quite different magnetic and magnetocaloric properties. The experimental outcomes are also compared with its bulk counterparts having disordered ferromagnetic ground state. Additionally, at the cryogenic temperature range, the significant magnetocaloric effect in both the samples indicate the applicability as a suitable magnetic refrigerant material. Moreover, the desertion nature of the magnetic hysteresis loop due to the field cycling indicates the superiority of the nanocrystalline compound over its bulk counterpart.

k0008
Effect of Chemical Pressure on the Structural, Magnetic and Thermodynamic Properties of DyVO4
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We report the results of structural, magnetic and heat capacity studies on Lu-substituted $DyVO_4$. No structural phase change is observed across the series; $Dy_{1-x}Lu_xVO_4$ (x= 0 - 0.4). Magnetic studies reveal the presence of metamagnetic transition within antiferromagnetic state of parent compound. The metamagnetic transition is getting smeared with Lu-substitution and suppresses completely for x – 0.4. Further, heat capacity data show that with increasing Lu-concentration, long range antiferromagnetic ordering temperature is decreased and Jahn Teller structural transition (~13 K for parent compound) vanishes completely.

k0009
Evolution of Crystal Structure and Magnetic Property with Cr Substitution in NiMnGa Alloy
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Based on first-principles DFT calculations, the magnetocrystalline anisotropy constant of NiMnGa in hexagonal phase is calculated to be -0.268 MJ/m3. The measured value of Curie temperature (TC) and saturation magnetization (Ms) of NiMnGa

is found to be ~400 K and 90.1 emu/g, respectively. The above observed properties make this material a potential candidate as rare-earth-free magnet for below room temperature applications. Further, our experimental work reveals that irrespective of the starting nominal compositions in NiMn1-xCrxGa, only ~15% Cr substitute the Mn atoms in the hexagonal NiMnGa phase and the remaining Cr segregate out in the bcc phase. With the increase in Cr concentration as the percentage of the hexagonal phase that primarily contributes to the ferromagnetic property is reduced, the TC and Ms values decrease, while the coercivity (Hc) and remanence (Br) values increase.

k00010

Muon Spin Relaxation Study of Ru-Based 6H-Perovskite, Ba3NdRu2O9

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The hexagonal perovskites $Ba_3RRu_2O_9$ (R = rare earth) consisting of Ru2O9 dimmers exhibits exotic ground states for various R-ions. In this family, the compound $Ba_3NdRu_2O_9$ orders ferromagnetically below 24 K (T_c) followed by another magnetic feature ~ 17 K (T_2), in-contrast to all other R-memebrs which shows antiferromagnetic ordering - this makes Nd-member intriguing. Here, we investigate the $Ba_3NdRu_2O_9$ compound using muon spin relaxation (μSR) to understand the spin-dynamics. We have collected the zero-field μSR data at ISIS facilities in UK. The muon asymmetry spectra were fitted with an exponential decay function. We observe a prominent λ peak and a significant drop in the asymmetry below the ordering temperature T_c). This confirms long-range magnetic ordering. However, we do not observe any other significant feature around 17 K which signifies that the magnetic feature around 17 K might be weak in nature and can be masked due to strong fluctuation of spin moments.

k0011

Correlation of exchange bias with negative magnetization in Gd2CoRuO6

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In the present work, we report negative magnetization (NM) and its correlations with exchange bias (EB) in Gd2CoRuO6 (GCRO). The GCRO compound crystalizes in P21/n space group, and has a magnetic ordering temperature (TC) of ≈ 60 K. The magnetization (M) vs temperature (T) curve under 50 Oe reaches its maximum value at 40 K, and shows the NM below the compensation temperature (Tcomp ≈ 10 K). The Tcomp is found to decrease with higher applied magnetic fields (H) and no NM is observed for H ≥ 500 Oe. Detailed investigation of M vs H curves reveals the presence of EB in the sample. The EB is found positive (also known as inverse EB) below the Tcomp whereas it is negative above Tcomp, indicating a connection between the NM and EB. Additionally, the values of coercivity and remnant magnetization, derived from the M (H) curves, show a minimum at the Tcomp. Such correlated magnetic behavior in GCRO has been understood from the temperature and magnetic field dependencies of Gd3+, Co2+, and Ru4+ sublattice magnetizations.

k0012

Influence of External Pressure on the Magnetic Ordering of 6H perovskite Multiferroic Material, Ba3HoRu2O9

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Understanding the influence of pressure to govern multiferroicity and ME coupling has great importance for the future realization of multiferroic devices. Here, we have investigated a fascinating multiferroic Ruthenate system, $Ba_3HoRu_2O_9$. The compound undergoes a long-range antiferromagnetic ordering at T_{N1} ~ 50 K, followed by another complex magnetic transition at T_{N2} ~ 10 K. Interestingly, along with strong re-orientation of Ho and Ru-spins, another new magnetic phase appears below T_{N2} consisting of (↑↑↓↓) spin-structure. Here, we report the effect of external pressure on magnetic ordering. It is observed that the magnetic peak temperature enhances gradually with increasing external pressure. For example, the magnetic peak at 10.4 K in the absence of external pressure shifts to 11, 11.5, and 12.2 K under the application of small pressure of 0.5, 0.8, and 1.2 GPa, respectively. These results manifest that the external pressure helps in magnetic ordering. In-contrast, the application of magnetic field decreases the magnetic ordering. We predict that 2nd-magnetic phase with (↑↑↓↓) spin-structure may be stabilized with application of external pressure and destabilized with application of magnetic field.

k0014

Magnetization Reversal and Domain Structures in Perpendicular Synthetic Antiferromagnets with Ir and Ru as Spacer Layers

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Ruderman-Kittel-Kasuya-Yosida (RKKY) coupling may occur between ferromagnetic (FM) layers separated by nonmagnetic metallic spacer layers, which could result in a stable synthetic antiferromagnetic (SAF) phase. Here, we have studied magnetization reversal by varying the number of bilayer stacks [Pt/Co] as well as thicknesses of Ir or Ru as spacer layers. In the first part we have studied various SAF structures having different Ir thickness (tIr) prepared on rigid Si (100) and flexible polyimide substrates. The sample with tIr = 1.0 nm shows a FM coupling, whereas sample with tIr = 1.5 nm shows an antiferromagnetic (AFM) coupling between the FM layers. At tIr = 2.0 nm, a bow-tie shaped hysteresis loop is observed indicating a canting of magnetization at the reversal. We have also demonstrated the strain-induced modification of IEC as well as the magnetization reversal phenomena. Further we discuss similar magnetization reversal study in SAF samples of Pt/Co layers with Ru as spacer layer. These samples show promising results which may be potential candidate for observing chiral spin textures.

k0015

Magnetic Phase Diagram of the Kitaev Honeycomb Antiferromagnet Single Crystal Na2Co2TeO6

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Spin systems with honeycomb structures have recently attracted a great deal of attention in connection with the Kitaev quantum spin liquid state (QSL) predicted theoretically. Here, we report the temperature and magnetic field dependent magnetic properties of one possible Kitaev QSL candidate $Na_2Co_2TeO_6$ realizing a honeycomb lattice of pseudo-spin-1/2. The isothermal magnetization curves measured at 2 K reveal strong anomalies correspond to field induced transitions at H_c ~ 57 and 60 kOe for H//a^* and H//a, respectively. In contrast, the magnetization for the H//c is found to be a very weak (~1/5 of that for H//a^* and H//a) with a slope change at 40 kOe. Therefore, the magnetic properties reveal a strongly anisotropic behaviours. We have determined magnetic phase-diagram for the applied fields along the high-symmetry directions (H//a, H//a*, and H//c) which reveal an anisotropic behaviour for the in-plane and out-of-plane directions. The present single crystal study shed light on the field induced magnetic phase transitions.

k0016

Double Transition Phenomenon and Magneto-transport Properties of Thick LCMO Film

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The magneto-transport properties of $La_{1-x}Ca_xMnO_3$ (LCMO) films with x=0.33, grown on STO substrate using the dc magnetron sputtering technique, were investigated in the presence and absence of a magnetic field. Electrical transport measurements shows that as we lowered the temperature, along-with a usual metal-insulator transition, 300 nm thick LCMO films shows a signature of additional transition which starts disappearing with increasing applied magnetic field. The magnetoresistance vs temperature (MR%-T) curves also exhibit two distinct peaks, which gradually merge into a single broad peak with increasing magnetic field. A range of temperature is observed for maximum MR% at 9 T magnetic field. This double transition phenomenon has been attributed to formation of charge-ordered antiferromagnetic insulator (CO-AFI) state which is suppressed by the application of the magnetic field. Magnetic measurements (M-T and M-H) curves also provide the signatures of the double transition phenomenon. At low temperature (below 40 K), an interesting resistivity upturn is also observed which is caused by dominance of CO-AFI phase over ferromagnetic-metal (FM) phase.

k0017

Complex Magnetism in Tetragonal Ho2Re3Si5

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We report the magnetic structure of tetragonal intermetallic compound $Ho_2Re_3Si_5$ using high-resolution neutron powder diffraction (NPD). The magnetic susceptibility, specific heat, and electrical resistivity showed two closely spaced

antiferromagnetic (AFM) transitions at T_{N1} ~3.8 K and T_{N2} ~ 4.2 K in $Ho_2Re_3Si_5$. The NPD patterns clearly show additional magnetic Bragg peaks with propagation vector k = (0 0 0) below T_{N1}, and k = (1/4 1/4 0) between T_{N1} and T_{N2} with respect to the tetragonal space group P4/mnc (128). The magnetic moments are pointing along the c axis below T_{N1} ~ 3.8 K, and along both a and b axes between T_{N1} and T_{N2} with up-up-down-down (UUDD) spin arrangement. The magnetic structure below T_{N1}, and between T_{N1} and T_{N2} is pure AFM exhibiting no net magnetization per unit cell. However, the net ordered site moment is found to be Ms = 9.06(3) μ_B/Ho at 1 K which is in close agreement with the saturated moment (M_s) of 9.2 μ_B/Ho obtained from the isothermal magnetization at 1.8 K. The $Ho_2Re_3Si_5$ also shows three field-induced metamagnetic transitions along the easy axis $\mu_0H \parallel c$ of magnetization. This study, therefore, reveals the magnetic ground state of this compound, which is essential to further explore the complex magnetic behaviour in the application of the magnetic field.

k0018

Tailoring the Structural and Magnetic Aspects of Zinc-Zirconium Substituted Strontium Hexaferrite System Targeting Diverse Applications.

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The study of phase evolution (with variation in calcination temperature) is critical in hexaferrite materials as their physical properties are significantly dependent upon the phase composition, which ultimately impacts their utility for various applications. M-type Strontium hexaferrite samples, $SrZn_xZr_xFe_{12-2x}O_{19}$ (x varying within 0.0 - 0.4) were prepared successfully using solid state reaction route. The influence of calcination temperature (900 °C – 1300 °C) on the physical properties of the pure (x=0.0) sample was explored. Rietveld refinement established that at 1300 °C, the pure sample develops preferred orientations along (006), (008) and (0014) crystallographic planes, whereas at 1200 °C, the phase purity for the samples $x \leq 0.3$ was confirmed. The presence of $ZnFe_2O_4$ and $SrZrO_3$ impure phases were observed in x=0.4 sample. M v/s H studies reveal an increase in M_s (90.26 emu/g (for x=0.0) to 91.41 emu/g (for x=0.1)) and a decreasing trend afterwards to 87.90 emu/g (at x=0.3). H_c value continuously decreases (5032 Oe (for x=0.0) to 1903 Oe (for x=0.4)). The magnetic data suggests that all the samples possess hard ferrite characteristics and could be useful for microwave absorbers, permanent magnets as well as spintronics.

k0019

Effect of Self-Doping on Magnetic and Magneto-Functional Properties of MnNiGe Alloys

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Magnetic equiatomic alloys of the form MM'X (M, M'= transition metals, X= Ge, Si, Sn, etc.) have caught the attention of researchers due to their innumerable magneofuntional properties, namely, exchange bias effect, sizeable magnetocaloric effect (MCE), etc., along with the shape memory property. Among several MEAs, MnNiGe alloy has been thoroughly investigated, which undergoes a structural transition of martensitic type, and a magnetic transition. Coupling these two transitions will lead to enriched properties. This can be achieved through various procedures, the most common being doping the alloy. So here we have presented structural and magnetic investigations of self-doped MnNiGe alloys of composition $Mn_{1.2}Ni_{0.8}Ge$ and $Mn_{1.22}Ni_{0.78}Ge$. The alloys are seen to undergo martensitic phase transition (MPT) from high-temperature (T) hexagonal to low-T orthorhombic structure, coupled with the MPT is a magnetic transition from paramagnetic to incommensurate antiferromagnetic nature with spiral modulation. Interestingly, at a magnetic field (H) of 1 kOe, a spin reorientation transition is observed from the a-axis to the bc-plane. MCE values are found to be 4.6 and 2.55 J/kg$^-$K for 70 kOe of changing H for $Mn_{1.2}Ni_{0.8}Ge$ and $Mn_{1.22}Ni_{0.78}Ge$ alloys, respectively.

k0020

Magnetic and Magnetocaloric Behavior of Ge-Doped Mn5Si3

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Ge-doped Mn_5Si_3 alloy of nominal composition $Mn_5Si_{2.98}Ge_{0.02}$ has been investigated through x-ray powder diffraction and dc magnetic measurements. The alloy crystallizes with a hexagonal structure with space group $P6_3/mcm$. Similar to the undoped Mn_5Si_3 alloy, on cooling from room temperature, this Ge-doped alloy also undergoes two magnetic transitions (paramagnetic ➔ collinear antiferromagnetic ➔ non-collinear antiferromagnetic). Dc magnetic data confirms a clear increase in collinear antiferromagnetic ➔ non-collinear antiferromagnetic transition temperature with Ge-doping. The unusual magnetic properties of the undoped Mn_5Si_3 alloy remain unaltered, and we have noticed a decrease in conventional and inverse magnetocaloric effects with Ge-doping.

k0021

Magnetic Anomalies in Nanocrystalline Dy4RhAl: Griffiths Phase like Behavior in Magnetic Susceptibility

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We report the results of dc susceptibility and heat capacity measurements on the (ball-milled) nanocrystalline rare-earth (R) ternary compound, Dy_4RhAl, crystallizing in Gd4RhIn-type cubic structure, containing three crystallographic sites for the rare-earth. While the results establish that the antiferromagnetic ordering observed in the bulk sample is suppressed with the reduction of particle size with no feature attributable to long-range magnetic ordering down to 1.8 K for the nanocrystalline form, the spin glass features get enhanced in the nanocrystalline form. Besides, the compound exhibits an inhomogeneous type of weak ferromagnetic component, characterized by a magnetic susceptibility behavior mimicking Griffiths -Phase.

k0022

Structural, Magnetic and Mössbauer Studies of X-Type Hexagonal Ferrites Sr2Co2GaxFe28-xO46

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X-type hexagonal ferrites $Sr_2Co_2Ga_xFe_{28-x}O_{46}$ (x = 0.0 - 2.0) have been synthesised by sol-gel auto-combustion method. The X-ray diffraction patterns confirmed that the pure X-type phase can be obtained by the calcinations at 1300 °C. The unit cell volume reduced from 2487.60 to 2465.25 $Å^3$ due to the smaller ionic size of gallium ion. The SEM analysis reveals agglomerated grains in the samples. The hysteresis loops showed a soft magnetic behaviour of all samples (coercivity between 8.45 to 9.5 kA m^{-1}). The saturation magnetisation was observed between 63 to 69 A m^2 kg^{-1}. Mössbauer spectroscopy confirmed the presence of Fe^{3+}-ions in the high spin state and the site occupancy of gallium ions at octahedral site (a↑).

k0023

Importance of V in the Magnetic Interactions in CrVO4

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Multiferroic materials exhibit spontaneous polarization (P) and magnetization (M) below the transition temperature. Type-II multiferroics, in particular, demonstrate simultaneous P and M arising from a robust coupling between spin and lattice degrees of freedom (DoFs), leading to intriguing magnetoelectric and magnetoelastic effects. Despite these exciting phenomena, the challenge remains in disentangling the contributions of these competing order parameters to tailor desired properties. To gain insights into the origin of P and M, temperature-dependent inelastic scattering measurements that track the behaviour of magnons and phonons across the transition temperature offer a rational approach. However, these spectroscopic techniques involve inherent complexities and uncertainties. To address these challenges, theoretical tools capable of selectively disentangling the relative contributions of quasiparticle excitations are needed. In particular, the impact of lattice DoFs (lattice strain and phonon eigenvectors) on other quasiparticles, such as magnons, remains underexplored in the existing literature. One such tool involves the theoretical extraction of orbital-resolved exchange interactions from the Hamiltonian using Green's and wannier functions. This approach enables a deeper understanding of the exchange mechanisms governing magnetic interactions and can be further investigated for controlling exchange interaction using ultrafast optical techniques. The potential applications of such research in the development of ultrafast sensors and detectors are promising.

k0024

Optical and Magnetic Studies on Single Crystalline 2D Van der Waals Compound, CrSiTe3

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We study the magnetic and optical properties of a novel two-dimensional Van der Waals material, $CrSiTe_3$ crystallizing in a rhombohedral structure with space group $R\bar{3}$. The results show ferromagnetic ordering around 33 K and an additional magnetic feature attributable to antiferromagnetic correlations and/or glassiness of the system. Raman spectroscopy data exhibit anomalous behavior with phonon softening below 100 K and signature of spin phonon coupling at the onset of magnetic ordering temperature.

k0025

Effect Of Y Doping On Magnetocaloric Properties Of Ho3Co

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The magnetocaloric effect of the rare earth rich intermetallic compounds of $Ho_{3-x}Y_xCo$ with x = 0.5 and 1 were studied in this work alongside a preliminary investigation on the magnetism of these two compounds. Upon nonmagnetic Yttrium substitution, the antiferromagnetic ordering temperature T_N was decreases by 21% and 33% for x = 0.5 and 1, respectively, from x = 0. The low temperature spin reorientation transition temperature (T_{SR}) was washed away with 33% Yttrium substitution in x = 1. The isothermal change in magnetic entropy ($-\Delta S_M$) for the compound with x = 0.5 remained similar to the parent compound with x = 0 but 19% decrease was noticed for x = 1, even though the values of $-\Delta S_M$ (13.1 J/kg-K) and

RC were quite reasonable for a magnetic field change of 9 T. Quantitatively, refrigerant capacity values are quite large at 665 J/kg for x = 0.5, which reduces to 582 J/kg for x = 1 for a field change of ΔH = 9 T

k0027

The Magnetic Anisotropy in TbIrIn5

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Single crystals of $TbIrIn_5$ with the tetragonal crystal structure were grown using the flux growth method and studied by means of temperature and field-dependent magnetic measurements exhibiting strong anisotropy and antiferromagnetic ordering with a Neel temperature of 42.5 K. Tb-moment is found to be close to its free ion value. A metamagnetic transition is observed at H_m=107 kOe along the c-axis at 2K. Below 2.6K, we observe a signature of diamagnetic behavior typical of superconducting phase. Further studies are in progress to ascertain this finding.

k0029

Tuning surface magnetism of NiO/Ag(001) system by changing thickness and stoichiometry

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In the present work we have studied the surface antiferromagnetism of NiO thin film grown on Ag (001) substrate. To probe surface antiferromagnetism a very surface sensitive technique, namely LEED (Low energy electron diffraction) is used. The ½ order diffraction spots, purely originated from the magnetic super cell provide the information of antiferromagnetic surface ordering. We found there is strong dependency of surface Néel temperature (T_N) with NiO thickness which make us able to tune the surface antiferromagnetism of the system. Another interesting feature we observed in this strongly correlated antiferromagnetic system is that the stoichiometry of the surface can also tune the antiferromagnetic Néel temperature (T_N).

k0030

Structural and Magnetic Properties of Cu Substituted Cobalt Nanocrystalline Ferrites

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Nano sized copper substitute cobalt ferrite $Co_{1-x}Cu_xFe_2O_4$ (x = 0.00 to 0.20 in steps of 0.05) were synthesized by citrate gel auto combustion method. The as prepared powders were characterized by X-ray diffraction. An x-ray diffraction pattern of all samples shows single phase cubic spinel structure. Experimental lattice parameters were found to decreases with increasing of Cu^{2+} ions; this is ascribed to the difference in ionic radii of Cu^{2+} ions and Co^{2+} ions. The magnetic properties of copper substituted cobalt ferrite were studied by using Vibrating Sample Magnetometer (VSM). Saturation magnetization (except at x=0.20) decreases with increasing of copper substitutions explained by Neel's sub-lattices modals whereas coercivity follows reverse trend.

k0031

Studies of Spin Correlations in Spin-Chain Compound Ca_3LiRuO_6

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We report the structural and magnetic properties of quasi one-dimensional spin-chain compound Ca_3LiRuO_6, where spin-chains are made up of Ru^{5+} (d^3, S=3/2) and Li^+ ions. Rietveld refinement of both x-ray and neutron diffraction pattern at room temperature confirms single-phase formation in rhombohedral structure with space group $R\bar{3}c$. Our refinement shows that Li and Ru ions are located at the trigonal prism and octahedral site, respectively. Additional peaks in the neuron diffraction appears below 115 K indicating the presence of a long-range antiferromagnetic (AFM) ordering. The additional peaks can be indexed with propagation vector k = (0, 0, 0). In the magnetic structure, determined from the Rietveld analysis of neutron diffraction data, magnetic moments are aligned along the crystallographic a-axis and coupled antiferromagnetically along the c-axis. No depolarization of neutron has been observed down to 1.5 K, ruling out the presence of ferro/ferri-magnetic component of the moment.

k0032

Existence of geometric frustration and possible spin-glass state in metastable rocksalt -$Zn_xMn_{1-x}O$ solid solutions

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We report the temperature dependent magnetic susceptibility of metastable rocksalt phase of Zn0.5Mn0.5O prepared using high pressure and high temperature (HPHT) techniques. The value of the frustration parameter [$f(\frac{\theta_{CW}}{T_N}) \approx 16$] obtained from our measurements confirm the presence of geometric frustration. The bifurcation of zero-field cooled (ZFC) and field cooled (FC) curves strongly indicates the formation of possible spin-glass state in this system.

k0033

Structural and Magnetic Studies of $La_{2-x}Sc_xCoMnO_6$ Double Perovskite

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Synthesized Scandium (Sc) doped $La_{2-x}Sc_xNiMnO_6$ (x= 0.0 and 0.1) double perovskites using solid state reaction method. Single phase monoclinic crystal structure with P21 /n space group was observed for samples by powder x-ray diffraction at room temperature. The FESEM images shows uniform grain distribution and grain size increases for Sc content sample The Field-cooled (FC) temperature dependence of magnetization curves show two FM transitions for x = 0.0 at T_{c1} ~ 220 K, T_{c2} ~ 155 K and for x= 0.1 at T_{c1} ~ 215 K, T_{c2} ~ 145 K.

k0034

Magnetic Properties of Fe Substituted $CoCr_2O_4$: Implications on Structure and Coercivity

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Structure and magnetism of $CoCr_{2-x}Fe_xO_4$ (x = 0, 1 and 2) samples have been studied using room temperature X-ray diffraction and temperature and magnetic field dependent magnetization measurements. With increasing Fe content, it has been found that the magnetic ordering temperature increases while the nature of magnetic ordering also undergoes drastic changes. However, the highlight of the work is that the equiatomic composition (i.e., for x = 1 sample) exhibits lowest coercivity thus making it attractive for device applications. The study presents a method of controlling magnetic properties through substitution, making it possible to prepare materials suitable for desired applications.

k0035

Magnetic Properties of Rare Earth Rich Intermetallic Compounds of $Dy_{3-x}Y_xCo$

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The magnetic behavior of $Dy_{3-x}Y_xCo$ within $0 \leq x \leq 1.5$ were studied based on dc-magnetization measurements. The antiferromagnetic (AFM) ordering temperature, TN, for x = 0 is reduced gradually upon Yttrium substitution and 50% decrease in TN was seen for x = 1.5. The low temperature AFM -to AFM transition observed at TAF ~35 K in x = 0 was also noticed to shift to lower temperatures initially for lower Y concentrations up to x = 1 and subsequently gets completely washed away on further increase in Y substitution to x = 1.5. The Griffith's like signature seen at 65 K, well above TN, for x = 0, was found to be present only in x = 0.5 and disappears for higher Y doping. Positive value of θ_P is suggestive of presence of ferromagnetic interactions in these antiferromagnetic systems for all x. The saturation magnetic moments per Dy atom even at 9 T and 2 K is only around 50% of its free ion moment, thus indicating the magnetic structure of all the compounds remain in non-collinear spin configurations for all the investigated samples.

k0036

Construction Of Magnetic Phase Diagram Of Skyrmionic Material $Co_{6.5}Ru_{1.5}Zn_8Mn_4$ By A Quantitative Approach

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The β-Mn-type cubic chiral compounds $(Co_{0.5}Zn_{0.5})_{20-X}Mn_X$ (x = 0, 2, 4, 6) exhibit a skyrmion phase over a wide temperature range (150 K – 400 K) is of great interest for future application in spintronics. One of the compound of this class, $Co_8Zn_8Mn_4$ having complex magnetic phases below the ferromagnetic transition temperature (T_c). In this article, we report the magnetic and magnetocaloric effect (MCE) for 4d-Ru doped on 3d-Co site of $Co_8Zn_8Mn_4$ i.e. for $Co_{6.5}Ru_{1.5}Zn_8Mn_4$. The different magnetic phases have been analyzed by the qualitative studying of MCE and the low field intricate magnetic phase diagram of $Co_{6.5}Ru_{1.5}Zn_8Mn_4$ is generated by employing the quantitative criterion of phase transition from scaling of isothermal magneto-entropy change.

k0037

Study of Structure and Magnetic Properties of Fe2CrAl Heusler Compound

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Understanding correlations between structure and physical properties is a starting point to investigate a novel phenomenon occurring in Heusler compounds. There are many Heusler compounds which are theoretically predicted but experimental studies are lacking. One such compound is Fe2CrAl, which is theoretically predicted to be half metallic subjected to desired doping. This report is on the study of Fe2CrAl compound. Its structural and magnetic properties were characterized by employing x-ray diffraction, neutron diffraction and commercial magnetometer. Magnetization studies are showing that the transition is taking place over a broad temperature range and there are intriguing magnetic properties much below and above the ordering temperature. We are in the process to carry out further advanced characterizations such as specific heat, temperature dependent neutron diffraction etc. to understand crystal and magnetic structure along with magnetic properties in detail.

k0038
Influence of Samarium on Structural and Magnetic Properties of ZnFe2O4
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In this study, the structural as well as magnetic characteristics of Zn1-xSmxFe2O4 (x = 0 to 0.15 with 0.05 increment) compounds are investigated, and the results are presented. The materials were synthesized using a solid-state conventional reaction technique. The patterns of X-ray Diffraction revealed the cubic inverse spinel phase with space group $Fd\bar{3}m$ by Rietveld refinement. The lattice parameters, bond lengths, bond angles, and other properties were approximated using Rietveld refinement. The samples' homogeneity and stoichiometry were validated using energy-dispersive spectroscopic analysis. Magnetization measurements at ambient temperature disclosed the superparamagnetic behavior of the investigated samples.

k0039
Tuning of Light and Magnetic Field Dependent DC Transport Property Induced by Transition in Conduction Mode with Temperature in P-type Si (100)/NiFe2O4/C60/ZnO-rGO Heterostructure
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We report temperature variation of current-voltage (J-V) characteristics of p-type Si (100)/$NiFe_2O_4$/C_{60}/ZnO-rGO composite heterostructure device under illumination of 660 nm red laser light and under external magnetic field. The J-V characteristics curves are found to be non-linear which is attributed to the bias dependent energy barriers for charge transport at the $NiFe_2O_4$/C_{60} and C_{60}/ZnO-rGO interfaces. At 300 K, photocurrent generation under 660 nm red laser light and positive magnetoresistance under external magnetic field have been observed in this device. However, both the magnetic field response and optical response are found to vanish at 110 K. Such tuning of light and magnetic field responses with temperature may be attributed to the temperature dependent shifting of relative energy level alignments in the present device which results in a change in conduction mechanism through the heterostructure.

k0040
Study of Magnetic Properties and Domain Imaging in Co/Gd Multilayer Synthetic Ferrimagnets
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Rare earth(RE) and transition metal(TM) synthetic ferrimagnets (SFiM) and ferrimagnetic alloys are composed of two different antiferromagnetically (AFM) coupled ferromagnetic layers. The dominance of RE or TM elements mainly depends on the temperature and relative concentration of the elements. Due to inequivalent magnetic atoms with different spin densities and lande g-factor, including antiferromagnetic coupling, this system offers excellent net magnetization and angular momentum tunability. The finite Zeeman coupling and spin polarization in these ferrimagnet systems is crucial in forming domain walls (DW) and its current-induced motion . Many exciting features, such as all-optical magnetization switching and high-speed domain wall motion , have been observed in these materials. The previous studies have been focused extensively on alloy-based ferrimagnets , however, recently, multilayer based SFiM have garnered more attention due to some of the distinct advantages such as easier growth process, easy tuning of properties by changing FM thickness, better engineering of the interfaces and robustness to thermal annealing, etc. . We have fabricated synthetic ferrimagnetic (SFiM) thin films with repetition of Co and Gd layers :$[Co(0.6)/Gd(t)]_3$ (unit: nm). All the films show perpendicular magnetic anisotropy with broken structural inversion symmetry at the interfaces. We have studied the magnetic properties and domain structures as a function of Gd thickness. Bubble domains have been observed for the sample with t_{Gd}=0.4nm whereas no domains have been observed for the sample with t_{Gd}=0.8nm. It is observed that by increasing the Gd thickness, the saturation magnetization of the samples decrease which indicates the enhancement of ferrimagnetic coupling between Co and Gd. Further, the FiM behavior has been confirmed via M-T measurements.

k0041

The Title Goes Investigation of Magnetocaloric Effect in Polycrystalline Spinel oxide $ZnFe_2O_4$

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$ZnFe_2O_4$ spinel has an interesting system for studying magnetic, electrical, thermoelectric and catalytic properties since they are strongly correlated to the crystal structure, particle shape, size and site substitution. In this work, solid state reaction has produced single phase, polycrystalline spinel oxide $ZnFe_2O_4$ (Cubic, Fd-3m). Data on magnetization vs temperature obtained in a field of 5 kOe reveal an antiferromagnetic ordering at 15 K. Curie-Weiss behaviour can be seen in the paramagnetic susceptibility. Magnetocaloric effect (MCE) has been evaluated in terms of isothermal magnetic entropy change (ΔS_m). The maximum value of ΔS_m is about 1.1 $Jkg^{-1}K^{-1}$arround transition temperature for a field change of 70 kOe. Here we report the magnetocaloric properties of bulk $ZnFe_2O_4$ sample.

k0042

Magnetization and Structural Study of Distorted Honeycomb Alternating Spin Chain Compound $Na_2Cu_2TeO_6$

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We report structural and magnetic properties of $Na_2Cu_2TeO_6$, a spin dimer compound. The single-phase polycrystalline $Na_2Cu_2TeO_6$ was synthesized using conventional solid-state reaction method. To analyze the crystal structure and magnetic behavior, we employed various characterization techniques. The crystal structure and magnetic properties are studied using X ray diffraction, Neutron Diffraction, and Magnetization measurements respectively. Structural study revealed that compound adopts a monoclinic crystal structure within the space group C2/m. It was also understood that $Na_2Cu_2TeO_6$ is composed of Cu_2TeO_6 layers, with Na atoms occupying the octahedral voids between these layers. Magnetization measurements were performed to study the compound's magnetic properties. The temperature-dependent magnetization measurements revealed a broad maximum occurring at 160 K, which is attributed to short-range 1D antiferromagnetic correlations. We are conducting temperature-dependent neutron diffraction studies to gain a deeper understanding of the magnetic structure of the title compound. The results from these studies will enable us to establish a microscopic correlation between the physical properties and the crystal structure.

k0043

Studies On Dextran Coated Fe_3O_4 Magnetic Nanoparticles For Simultaneous Magnetic Fluid Hyperthermia And Release of Imidazole

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Dextran coated Fe_3O_4 magnetic nanoparticles (MNPs) were synthesized using a coprecipitation technique. To probe simultaneous magnetic fluid hyperthermia and magneto-thermal drug release, these particles were loaded with imidazole. The imidazole molecules were bound to dextran through hydrogen bonding, which was reversible. The encapsulation efficiency decreased with increasing particle concentration due to agglomeration induced lowering of surface active sites. The magnetic nanoparticles exhibited superior field induced heating efficiency, and magneto-thermal drug release was activated beyond ~ 40 ^oC, which is therapeutically relevant. The studies clearly showed the efficacy of dextran coated Fe_3O_4 MNPs for simultaneous magnetic fluid hyperthermia and magneto-thermal drug release applications.

k0044

Study of Y-type $Ba_{0.5}Sr_{1.5}Co_{1.5}Mn_{0.5}Fe_{12}O_{22}$ hexaferrite

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A sample of $Ba_{0.5}Sr_{1.5}Co_{1.5}Mn_{0.5}Fe_{12}O_{22}$ Y-type hexaferrite was synthesized using the sol–gel method. A Y-type hexagonal phase structure was confirmed by XRD analysis. The grains are plate-like in shape, according to a scanning electron micrograph (SEM) of the sample. Mossbauer measurements were used to determine the distribution of Fe3+ ions in the sample. Changes are observed in Raman spectra and bulk magnetization as compared to the parent sample i.e., $Ba_{0.5}Sr_{1.5}Co_2Fe_{12}O_{22}$.

k0045

Effect of Ni Substitution on Intrinsic Magnetodielectric and Magnetic Transition of $Ba_2Mg_2Fe_{12}O_{22}$ Hexaferrite

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We have synthesized the polycrystalline $Ba_2Mg_2Fe_{12}O_{22}$ (BMF) and $Ba_2Mg_{1.5}Ni_{0.5}Fe_{12}O_{22}$ (BMNF5) hexaferrites using well known solid-state reaction method. The modifications in crystal lattice parameters, magnetic, and magnetodielectric properties, upon Ni substitution in BMF, have been investigated. Ni^{2+} substitution at the Mg^{2+} site in BMF enhances the conical spin ordering temperature (T_I) from 35 to 52 K. A step-like variation in magnetization with applied field suggests possible intermediate magnetic field induced spin configurations. The magnetic field-dependent dielectric constant (ε_r') and dielectric loss (tan δ) at room temperature indicate the magnetodielectric (MD) effect in both samples. Interestingly, the intrinsic MD effect is found to be in a large frequency range (10k Hz ≤ f ≤ 1 MHz) for BMNF5 in comparison to less frequency range (100k Hz ≤ f ≤ 1 MHz)) for parent BMF.

k0046

Comprehensive Analysis of the Structural Properties of Zr-Doped $TbMnO_3$ Manganites

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Zirconium-doped $TbMnO_3$ with the chemical formula $TbMn_{1-x}Zr_xO_3$ (where x = 0.00, 0.05, 0.075, 0.1) were synthesized using the conventional solid-state method. The crystal structure analysis using X-ray diffraction revealed that all samples maintained the orthorhombic structure, and the doping caused compression of the unit cell, resulting in changes in the cell parameters and volume. Additionally, room temperature Raman spectroscopy showed six active modes, with slight frequency shifts observed after Zr-doping. The substitution of Zr on the Mn site in $TbMnO_3$ resulted in a reduction in grain size as evidenced by FESEM micrographs, with respective values of 6.401 µm, 4.697 µm, 4.057 µm, and 3.785 µm for x= 0.00, 0.05, 0.075, and 0.1.

k0047

Structural and Magnetization Study of Yb_2CoMnO_6 Double Perovskite Compound

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Double perovskite compounds have shown intriguing physical properties owing to numerous possibilities of placing ions at various sites. Here double perovskite Yb_2CoMnO_6 compound have shown magnetic field induced modification in magnetic structure, which lead to alter physical properties significantly. We intend to focus on identifying the microscopic origin of the phenomenon through magnetic structure studies. The title compound was synthesized by solid state reaction method. The phase purity of synthesized sample has been studied by x-ray diffraction and neutron diffraction under ambient conditions and it was found to be crystallized in monoclinic crystal structure with space group **$P2_1/n$ (sg#14).** The temperature and magnetic field dependent magnetization was studied by employing the vibrating sample magnetometer (VSM) attached with commercial physical property measurement system (PPMS) to ascertain magnetic properties, which indicates magnetic transition around 48 K. T The temperature dependent neutron diffraction and other physical characterizations like magneto-dielectric study are being studied to understand multifunctional behavior in title compound.

k0048

Cross-correlations between Spin-Lattice Degrees of Freedom in Two Magnetic Sublattices of $Li_{0.5}Fe_{2.5-x}Cr_xO_4$ across Magnetic Compensation

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In recent times, magnetic phenomena like magnetic compensation, spin reorientation, etc., in complex oxides have gained much importance due to their practical applications in spintronics device fabrication. These phenomena occur due to coupling between electronic spin and phonons in a lattice. Here, we investigate the strong interlinkage of electronic spin and phonon in $Li_{0.5}Fe_{2.5-x}Cr_xO_4$ (x = 1.1, 1.3, 1.5, and 1.6) across the magnetic sublattices (of octahedral and tetrahedral symmetries) showing magnetic compensation. Temperature-dependent micro Raman studies reveal anomalies in phonon wavenumber with temperature below the spin ordering temperature. The Fano line-shape of the phonon mode of the tetrahedral site also helps to understand the linkage of a phonon with electronic spin. This study reveals a complex interplay between spin and lattice degrees of freedom in $Li_{0.5}Fe_{2.5-x}Cr_xO_4$.

k0049

Structure, Stability and Magnetic Properties of Perovskite Type $Ba_2Fe_{1.33}U_{0.67}O_6$

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Herein we report the structure, stability and magnetic properties of perovskite type $Ba_2Fe_{1.33}U_{0.67}O_6$ and $Ba_2Fe_{1.33}U_{0.67}O_{6-\delta}$ compositions prepared by solid state reaction. The compound crystallizes in the cation ordered cubic (Fm-3m) perovskites structure. The structure remains stable on reduction at moderate temperature while at higher temperature and prolonged

reduction it decomposes to metallic iron and Ba_3UO_6. The magnetization studies on the pristine and reduced perovskite phase show ferrimagnetic transition and the transition temperature is found to be lower in reduced sample compared to their pristine analogue. Field dependent magnetization measurements indicate almost no coercivity suggesting soft-ferromagnetic nature for both samples.

k0050

Probing structure-orbital correlation for high-Tc $PrOFe_{0.9}Co_{0.1}As$

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Correlation between structure of $FeAs_4$ and Fe 3d electron itineracy was investigated for $PrOFe_{0.9}Co_{0.1}As$, with XRD and As K-edge XANES techniques. Tetrahedral size of $FeAs_4$, rather than angle, was determined to be most effective in manipulating electron orbitals. These results provide realistic evaluation of the structural control of transport in high-Tc pnictide superconductors in general.

k0051

Structure and Magnetic Properties of New Tetragonal High Entropy Spinel Oxides

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Two new high-entropy spinel oxides, with composition $(Mn_{0.2}Co_{0.2}Ni_{0.2}Cu_{0.2}Zn_{0.2})Mn_{1.8}Cr_{0.2}O_4$, $(Fe_{0.2}Co_{0.2}Ni_{0.2}Cu_{0.2}Zn_{0.2})Mn_2O_4$ has been successfully synthesized using the solid-state synthesis method. The room temperature X-ray diffraction, Scanning Electron Microscopy, and Energy Dispersive Spectroscopy analysis highlight that the samples are crystalized in a tetragonal spinel structure with excellent chemical homogeneity at the microscale. The temperature and magnetic field-dependent magnetization studies revealed a complex magnetic behavior characterized by a ferrimagnetic ordering followed by a noncollinear magnetic ground state at lower temperatures. Interestingly, $(Fe_{0.2}Co_{0.2}Ni_{0.2}Cu_{0.2}Zn_{0.2})Mn_2O_4$ shows a huge coercive field (H_C) of 1.1 T. Our study demonstrates the feasibility of incorporating multiple elements within a complex tetragonally distorted oxide structure. This opens up exciting possibilities for designing and customizing properties in correlated and quantum materials.

k0052

Influence of Induced Anisotropy on Magnetoimpedance in Electrodeposited Trilayer Films

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Investigating interaction effects in FM/NM/FM (ferromagnetic/spacer/ferromagnetic, spacer: non-magnetic or ferromagnetic) trilayer films electrodeposited on a Cu wire substrate (diameter: 0.1mm) is the focus of this study. We explore magnetoimpedance (MI) phenomena to elucidate induced anisotropy's impact on giant magnetoimpedance (GMI) behavior. Our findings reveal that MI profile characteristics are influenced not only by the magnetization direction within each magnetic layer but also by the positioning of the magnetic layer along the non-magnetic wire. This behavior arises due to the presence of longitudinal or transverse anisotropy in one of the layers, adding a new dimension to the understanding of GMI responses.

k0053

Lack of Evidence for Topological Superconductivity in Pd Intercalated $NbSe_2$

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Topological superconductors have garnered considerable research interests in the past two decades. Being the host of Majorana bound states, which can pose as qubits, these materials can provide robust grounds for the development of quantum computation. Here, we report effect of Pd intercalation in $NbSe_2$, which is a well-known superconductor as well as a potential candidate to exhibit topological superconductivity. These compounds are examined using the structural, magnetic measurements and penetration depth measurement which is a powerful and the most sensitive tool to detect the pairing symmetry of superconductors. Structural characterization reveals successful intercalation of Pd atoms. Our results show that 10% Pd intercalation in $NbSe_2$ suppresses superconductivity. Penetration depth measurements indicate towards the two-gap superconductivity in the sample.

k0054

Tailoring Exchange Bias in Core-Shell (Ni-NiO) and Inverse Core-Shell (NiO-Ni) Structure

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This article reports studies of exchange bias (EB) in core-shell Ni-NiO and inverse core-shell NiO-Ni structures. In regular core-shell, ferromagnetic (FM) Ni resides in the core and antiferromagnetic (AFM) NiO shell surrounds the core. The structure is altered in inverse core-shell. Nanostructured Ni-NiO and NiO-Ni are synthesized via controlled oxidation-reduction in wet chemical route. Samples are characterized with powder X-ray diffraction (PXRD) studies. Magnetic hysteresis loops (M-H) in field-cooled (FC) mode for both the samples show a shift along the field axis followed by increase in coercivity – a signature

mark of exchange bias effect. A third sample with 50:50 weight percentage of well mixed Ni-NiO:NiO-Ni could not enhance the EB significantly.

k0055

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.

k0056

Order Parameter Symmetry in Superconducting 2H-TaSeS

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Tantalum based transition metal dichalcogenides are prime members of topological superconductors, which significantly correlate with charge density wave (CDW) ordering as well. Here, we have carried out an in-depth investigation of transport measurements in high-quality single crystals of TaSeS. We have obtained superconducting transition temperature (T_c) which is 4.15 K, which is among the highest recorded T_c in the system $TaSe_{1-x}S_x$. Additionally, there is evidence of charge density wave onset at 66K. Moderate anisotropy with a value of 1.52 was seen in upper critical fields. With a considerable superconducting energy gap of around 1meV, radio frequency penetration depth measurement reveals that the superconductor TaSeS has s-wave pairing in the moderately strong coupling limit.

k0057

Spin-Phonon Coupling through Multiple Magnetic Phase Transitions and Orbiton Mediated Multiphonon Scattering in Infinite-Layer $La_{0.875}Sr_{0.125}MnO_3$

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The infinite-layer $La_{1-x}Sr_xMnO_3$ perovskite manganite is a member of the Ruddlesden-Popper series (La, Sr) $_{m+1}Mn_mO_{3m+1}$, where m=∞. The recent discovery of skyrmionic bubble formation and the phenomenon of colossal magnetoresistance in this system draws special attention. In this work, we have studied the orthorhombic infinite layer -$La_{0.875}Sr_{0.125}MnO_3$ (IL-LSMO-0.125). The compound shows several magnetic and electrical phase transitions with temperature. We perform temperature-dependent micro-Raman measurements between 80K and 300K, over which the system evolves from a ferromagnetic insulating (FM-I) to a paramagnetic insulating (PM-I) phase after passing through a ferromagnetic metallic (FM-M) and a canted antiferromagnetic insulating (CAFM-I) phases. The analysis of the spectra reveals non-monotonic behavior in Raman shift vs. temperature plots of the first-order phonon modes across magnetically ordered phases. This observed anomalous softening of the Raman shift indicates complex spin-phonon coupling across multiple magnetic phases. The unusual variation of Raman spectral line width with temperature across metal-insulator transition (MIT) has been demonstrated. The distinct correlation between the orbiton-related phonon modes and first-order Raman modes at low temperatures indicates the presence of orbiton-polaron in determining the FM-I phase of the compound.

k0058

Magnetic and exchange bias properties in Pr_2NiIrO_6

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Polycrystalline double-perovskite Pr_2NiIrO_6 sample was synthesized using solid state reaction. X-ray diffraction measurements indicated that the sample exhibited a monoclinic crystal structure with space $P2_1/n$ group. The temperature and field variation of magnetic measurements indicated that Pr_2NiIrO_6 sample showed ferromagnetic like behavior at low temperature and paramagnetic behavior at room temperature. The field cooling magnetization- magnetic field hysteresis curve showed exchange bias properties in the prepared sample. The exchange bias properties would be originated from the Dzyaloshinsky-Moria interactions. The iridium (Ir) based double perovskite Pr_2NiIrO_6 sample exhibited an interesting magnetic properties in the present study.

k0059

The Investigation of Structural and Magnetic Properties of spin-chain oxide Li_3RuO_4

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We studied the structural and magnetic properties of the disorder free quasi-one-dimensional zig-zag spin-chain compound Li_3RuO_4. Rietveld refinement of room temperature x-ray and neutron diffraction data confirms the single-phase formation of the compound Li_3RuO_4 in an ordered rock-salt structure (space group P2/a). Additional peak in the neuron diffraction pattern appears at low temperature, indicating an onset of long-range magnetic ordering. No depolarization of neutron beam has been observed down to 4K, ruling out the presence of ferromagnetic correlations.

k0060

Improved Magnetic and Dielectric Properties in La Doped $BiFeO_3$

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$BiFeO_3$ and $Bi_{0.80}La_{0.20}FeO_3$ samples were prepared by the traditional solid state reaction technique. Both samples crystallized in rhombohedralR3ccrystal structure, as was evidenced from their X-ray diffraction patterns. The scanning electron micrographs indicated that grain size of $BiFeO_3$ sample was reduced with the substitution of La. The magnetization and coercive field are improved in $Bi_{0.80}La_{0.20}FeO_3$sample. The frequency variation of dielectric data showed that the samples exhibited dielectric relaxations in the measured frequency range. The enhanced magnetic and dielectric properties were observed in the La substituted $BiFeO_3$sample.

k0061

Crystal Structure and Magnetism of $Gd_{1-x}Y_xNi$ (x = 0, 0.25, 0.5, 0.75) Rare Earth Intermetallic Compounds

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Rare earth intermetallic compound GdNi (Orthorhombic, CrB-type) is a ferromagnet with an ordering temperature of 69 K (T_C). Interesting magnetoelastic and magnetocaloric effects are observed near T_C [1, 2]. Effect of non-magnetic yttrium substitution at Gd-site on the crystal structure and magnetism has been studied in this work. In most of the rare earth- nickel based intermetallic compounds, Ni 3d band is full and Ni does not contribute to magnetism. X-ray magnetic dichroism studies on GdNi compound revealed a small induced moment at Ni-site [3]. The samples $Gd_{1-x}Y_xNi$ (x = 0.25, 0.5, 0.75 and 1) were prepared by arc-melting and were characterized by powder X-ray diffraction and dc magnetization measurements. The compounds $Gd_{1-x}Y_xNi$ with x = 0.5 and 0.75 have orthorhombic FeB-type crystal structure (space group Pnma, no. 62) and order ferromagnetically around 62 K and 22 K respectively. The end member YNi has the same orthorhombic FeB- type structure at room temperature and it is a Pauli paramagnet. The change in the T_C and saturation magnetization values with increase in Y content seems to imply that Ni does possess a weak magnetic moment that couples antiparallel with the 4f Gd moment in these systems.

k0062

Enhancement in Critical Current Density and Strong Pinning Superconducting Phase Found in a High Tc Superconductor - Transition Metal Carbide Nanocomposite

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The superconducting properties of pelletized nanocomposite materials comprised of the powders of Bi-2223 and Co_2C are explored here. The system loses over 97% of their superconducting portion, but the remaining 3% still displays strong bulk superconducting properties. The fraction's T_c~109 K, approximately equals to that of the pure Bi-2223 pellet. The contributions from the ferromagnetic and superconducting fractions are superimposed in the composites' net magnetization response. Also a strong Meissner reaction is present in the remaining superconducting portion. The superconducting fraction's irreversibility field at 77 K is observed to rise by roughly three times compared to the parent system, exhibiting strong vortex pinning characteristics. Also a Broadened magnetic field regime over which we observe a single vortex pinning regime sustained in the nanocomposite. The critical current density, J_c, of the nanocomposite approximately five times higher than the pristine Bi-2223 pellet at low T and the enhancement in J_c is most significant in the high T regime, where we see almost two orders of magnitude increase of J_c compared to the pristine Bi-2223 pellet, which is important for high current applications.

k0063

Magnetic properties of non-centrosymmetric $PrAlSi_{1-x}Ge_x$ (x = 0, 0.05, 0.1) compounds

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The ternary $PrAlSi_{1-x}Ge_x$ (x = 0, 0.05, 0.1) compounds, which crystallized in tetragonal LaPtSi-type structure (space group $I4_1md$) were prepared by arc melting and characterized using powder x-ray diffraction, magnetization, resistivity/magnetoresistance, and heat capacity. Magnetic susceptibility $\chi(T)$ of all the compounds shows ferromagnetic-like ordering with a drop at low temperatures. Heat capacity measurement confirmed the long-range order and presence of the f-level splitting due to crystal field effect. All the compounds' resistivity data indicate metal-like behavior and shows large positive magnetoresistance.

k0065

Structural and Multi-Phase Magnetic Behavior of Pr_2NiMnO_6 Double Perovskite

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In the last few years, rare-earth-based double perovskite R_2NiMnO_6 (R = rare earth element) has attracted attention because of its intriguing physical characteristics and prospective usage in spintronic devices. La_2NiMnO_6 is already known for its room temperature multiple physical properties but there is little in-depth knowledge of the magnetic ordering in Pr_2NiMnO_6 when compared to considerable investigations on the characteristics of bulk materials. In our prepared Pr_2NiMnO_6 sample, a monoclinic crystal symmetry obtained with the space group $P2_1/n$ and temperature-dependent magnetization M(T) data shows a transition at 212K which is associated with the ferromagnetic ordering of Ni^{2+}-O^{2-}-Mn^{4+}. Additionally, the presence of a spin cluster state was observed at low temperatures in the M(T) data, which was further confirmed by the AC Susceptibility measurement. A downturn in M(T) measurement at lower temperature suggests that the Pr^{3+} and Ni-Mn sublattice are antiferromagnetically coupled. The magnetocaloric effect measurement on negative entropy change, however, shows that the application of a stronger magnetic field will move the Pr^{3+} moment parallel to the Ni-Mn sublattice.

k0066

Absence of Universality in Linear Resistivity of Cuprates

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The understanding of "strange" metallic state that is characterized by linear temperature dependent resistivity up to the highest measured temperature in copper oxide based high temperature superconductors (HTSC) is one of the major challenges in condensed matter physics. The relation between superconducting transition temperature (T_c), doping level (x) and the T-linear coefficient ($A^{\square}_1$), as $T_c \sim (x_c\text{-}x)^{0.5} \sim (A^{\square}_1)^{0.5}$ has been reported [1], where x_c is the critical doping at which superconductivity disappears and $A^{\square}_1$ is the coefficient of the linear resistivity per CuO2 plane. But we have observed contradiction to this scaling laws in Zn-doped $La_{2-x}Sr_xCuO_4$, Fe-doped $Bi_2(Sr_{0.6}Ca_{0.4})_3(Cu_{1-x}Fe_x)_2O_y$ and electron irradiated $YBCO_7$ ($YBa_2Cu_3O_{7-\delta}$) in which T_c can be varied without doping [2,3,4]. We have shown that T_c does not depend on $A^{\square}_1$ in these system violating the proposed universal scaling laws.

k0067

On the Experimental Evidence for Possible Superconductivity in LK 99

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The desire to create an energy efficient world is bound to be incomplete without the discovery of a room temperature superconductor at ambient pressure. The recent report on the room-temperature ambient-pressure superconductor has inspired scientists to study the Cu doped Lead Apetite named as LK-99. Here, we have synthesized Cu doped LK-99 and Ni-doped LK-99 compounds and studied their temperature dependent transport and magnetization behaviour. The temperature dependent resistivity clearly shows the insulating nature of the sample. The temperature dependent penetration depth measurement unveils the absence of superconductivity in this sample. The temperature dependent ac susceptibility measurement reveals the paramagnetic nature of the Ni doped LK-99.

k0068

Structural and Magnetic Properties of Sr_2NiMO_6 (M=W,Mo)

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Here, We report the Structural and magnetic Properties of double perovskite Sr_2NiMO_6(M=W,Mo). The Polycrystalline samples Sr_2NiMoO_6 (SNMO) and Sr_2NiWO_6 (SNWO) were synthesized using Solid state reaction method. By employing X-ray powder diffraction and Rietveld analysis, we unveiled that both SNMO and SNWO samples adopt a tetragonal structure with the I4/m space group.. Temperature dependence of magnetization measurement determined that both SNMO and SNWO samples undergoes the transition from paramagnetic to antiferromagnetic transition around 74.2K and 58K respectively. Upon subjecting both samples to a magnetic field, an antiferromagnetic nature is evident. Notably, SNMO exhibits an additional ferromagnetic nature at lower temperature. We also have fitted Modified Curie-Wiess law from which we got Curie temperature are -254.59K and -160.5K, and effective magnetic moment(μeff) are 4.18 μ_B/f.u. and 3.8 μ_B/f.u. for both samples

SNMO and SNWO respectively. These comprehensive insights contribute to a deeper understanding of the magnetic behaviors exhibited by SNMO and SNWO.

k0069

Hypothetically Predicted Fe_2CoS and Ni_2CoS Alloys for Spintronics Applications: A DFT Study

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The ground state properties of the newly predicted full Heusler alloys Fe_2CoS and Ni_2CoS were computed using first principles calculations. The basis set of well-known FP-LAPW is used in the computations. The GGA-PBE functional is used to address exchange-correlations. According to the electronic calculations, these alloys have a bandgap in the majority state and metallic behavior in the minority state, which indicates that they are half-metallic ferromagnets. The bandgap findings match the results of the DOS. The magnetic moments of the Fe_2CoS and Ni_2CoS alloys are computed, indicating half metallicity and strong spin polarization for these full Heusler alloys. The investigated alloys are suitable for spintronics applications.

k0070

Parameter Selection of Amorphous Magnetic Core for Linear Transformer Driver (LTD)

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A magnetic core is an important component of Linear Transformer Driver (LTD) pulsed power generator which acts for isolating main current from diverting to unwanted return current path. The efficiency of LTD output depends on impedance offered by these magnetic core in current return path. Here we have explained design and testing of magnetic cores being used in our LTD development.

k0071

On Thermomagnetic Irreversibility in $CoS_{2-x}Se_x$

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The path dependence of paramagnetic (PM)-ferromagnetic (FM) transition in $CoS_{2-x}Se_x$ (x = 0.24, 0.26, 0.28) is investigated in magnetic field-temperature space. We show a re-entrant transition from PM to FM followed by FM to PM for these compositions when the sample is warmed in the presence of a magnetic field after zero-field cooling. By following different paths in H-T space, we show that PM state is the non-equilibrium state for these compositions which transform to FM state on warming.

k0072

Study of Magnetocaloric Effect and Magnetoresistance in Mn Substituted FeRh

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The influence of Mn substitution on the first order antiferromagnetic to ferromagnetic transition in FeRh has been investigated. The magnetization measurement suggests that Mn moments align parallel to Fe moment. In the AFM region, the isothermal magnetization shows ~3% residual magnetization. The temperature dependence of resistivity and magnetization show that transition temperature is shifted to near room temperature. It results in a giant magnetocaloric effect (~14 J/Kg-K) and a large magnetoresistance (~-40%) for a magnetic field change of 50 kOe around room temperature. The working range of MCE and MR is shown to be dominated by transition broadening.

k0073

Role of Vanadium Doping over T_C and Upper Critical Field of the Non-Centrosymmetric Superconductor, NbReSi

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In this paper, we report the role of non-magnetic vanadium impurity (0 to 5%) on the superconducting properties of the non-centrosymmetric superconductor, NbReSi. Initially, a powder X-ray diffraction (XRD) analysis of $Nb_{1-x}V_xReSi$ (x = 0, 0.015, 0.025, 0.05) was carried out at ambient temperature and pressure for the identification of the single-phase and structural configuration of the prepared samples. Furthermore, Rietveld analysis of the XRD data confirmed the preserved orthorhombic crystal symmetry in all the compositions and a consistent change in lattice parameters in the doped variants (a uniform decrease in the 'a' direction and a consistent increase in the 'b, c' directions are observed). However, the lattice parameters of the parent samples exhibited a consistent result with the published literature. In addition, a comprehensive study of the resistivity measurements of pristine and doped samples with the variation of field and temperature was performed to investigate the role of vanadium doping over the upper critical field ($\mu_0 H_{c2}$) and suppression of T_c. A monotonic decrease of T_c was observed with the increase in doping percentage. In this analysis, $\mu_0 H_{c2}$ was determined at the mid-value of ρ_N, which yields [$\mu_0 H_{c2}(0)$].

A uniform reduction of [$\mu_0 H_{c2}(0)$] was also found with an increase in impurity percentage. Interestingly, [$\mu_0 H_{c2}(0)$] was found to surpass the weak-coupling Pauli limit for pristine and doped variants (up to 2.5%).

k0074

Structural and Magnetostrictive Properties Of Y3+ Substituted CoFe2O4

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We report the effect of yttrium (x=0.00, 0.01, 0.03 and 0.05) substitution on the structural and elastic properties of cobalt ferrite ceramic synthesized by solution combustion route. All synthesized samples were sintered at 1200°C for 10 hr. The refined XRD patterns for all composition confirm the formation of single-phase of spinel ferrite. The microstructure was examined by using scanning electron microscopy. The XRD study confirms the formation of single-phase cubic spinel lattice. The FTIR spectra study confirms spinel phase formation. We have calculated force constant from FTIR spectra. For composition, x=0.03, the high value of strain sensitivity ~ 0.14 ppm/Oe is observed at lower magnetic field. The maximum magnetostriction coefficient~183 ppm is observed for composition x=0.05. The obtained high value of strain sensitivity x=0.03 is useful for making the magnetoelectric based energy harvesting composites.

k0075

Effect of substitutional doping on Fe-based superconducting series: interplay of magnetism and superconductivity

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Over the last decade, the superconducting series based on Fe-chalcogenides has retained the relevant focus because of their multitudes of strongly correlated attributes like coexisting magnetic and superconducting phases and their interplay with multiple structural transitions leading to panoply of complex phase-diagrams. In the present work, with the help of low-temperature magnetization measurements and first-principles theory, we have investigated the role of both cationic and anionic substitution on the correlated behaviour of the series FeSe, FeTe, FeSeTe and CuFeTe. First-principles density-functional calculations imply that all four systems are stabilized in a tetragonal symmetric structure with A-type antiferromagnetic spin-arrangements. Low-temperature magnetic measurements indicate that the superconducting properties of FeSe are less supressed with anionic Te substitution than the cationic Cu substitution. We have analysed these results in the light of the substitution-induced modification of electronic properties.

k0076

Fabrication and Characterization of YBCO Step-Edge Josephson Junction on MgO Substrate

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Josephson junction is the key element of superconducting electronics such as highly sensitive magnetometers and voltage amplifiers, terahertz detectors and superconducting quantum computers, etc.
In this work, we have fabricated YBa2Cu3O7-x (YBCO) step edge Josephson junction on MgO substrate. Step on MgO substrate is created using mask aligner and ion beam milling (IBM) technique. Step on the substrate is characterized using atomic force microscopy (AFM) technique from which step height and step angle are found to be ~ 450 nm and ~ 14° respectively. The Film is deposited epitaxially along the c-axis on the MgO substrate using the pulsed laser deposition (PLD) technique. Josephson junction is created on the film using photolithography and IBM technique. The YBCO film is characterized using X-ray diffraction (XRD) and energy dispersive X-ray (EDX) spectroscopy techniques. The presence of (00l) peaks confirms the epitaxial growth of film along the c-axis of the YBCO film onto the substrate. The stoichiometry of the film is confirmed using the EDX measurement. The superconducting properties of YBCO film are characterized using resistance versus temperature (R-T) measurement, from which the critical temperature (Tc) of the film is found to be 86.2 K. The Josephson junction is characterized using current versus voltage (I-V) measurements. At 77 K, the critical current (Ic) and normal state resistance (Rn) of the junction are found to be 0.21 mA and ~ 0.86 Ω, respectively, giving the characteristic voltage (Vc = IcRn) to be around 0.18 mV which is better than previously reported values. This device has potential applications in the field of terahertz detection.

k0077

Effect of B-site Disorderness on Magnetic Transitions of Polycrystalline $SmCrO_3$ with Fe Substitution

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Rare earth orthochromites, $RCrO_3$ (R-rare earth ion) show interesting magnetic properties such as spin reorientation, magnetization reversal, large magnetocaloric effect (MCE), and multiferroicity due to complex exchange interactions and strong correlation to the spatial effect of ions at rare earth or Cr site. This work reports the magnetic properties of samarium-

ferrochromite $SmFe_{0.5}Cr_{0.5}O_3$ to understand the influence of B- site Fe doping, on magnetic transitions in $SmCrO_3$ and 3d-4f exchange interactions of magnetic sublattices. X-ray diffraction (XRD) confirms the phase purity with orthorhombic crystal structure and Pbnm spatial symmetry. Morphology investigation by scanning electron microscopy (SEM) evidences homogeneous well-defined grains. Magnetic investigations give Néel transition temperature (T_N) near 265 K, demonstrating a shift towards room temperature with diluting Fe^{3+} ions in $SmCrO_3$. The occurrence of spin reorientation just below T_N is estimated referring to previous work in ferrochromites and development of the ferromagnetic component in lower temperature regime is related to Sm^{3+} sublattice ordering and existing complex exchange interactions.

k0078

Microstructural and magnetic studies on Superconducting YBCO cylinder.

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High-temperature superconductors have paved path for new era of innovative technological advancement across various disciplines, ranging from transportation to communication, high magnetic field application to quantum computation. The applications of high-temperature superconductors are limited to simple shapes due to the ceramic nature of the superconductors and the influence of the process on the final property. The present work addresses this issue by exploring the integration of Preform Optimized Infiltration and Growth processing of YBa2Cu3O7-δ (YBCO) with a modified slurry-based process from a complex-shaped superconducting product. A cylindrical shape was fabricated to establish the potential of the fabrication technique as well as study superconducting properties. The superconducting cylinder shows superconducting transition around 92 K and current densities as high as 20 KA/cm2 at 77K, which sustained up to magnetic field of 5T. The initial studies on superconducting cylinders are promising and can realize the development of complex-shaped superconducting components for various applications.

k0079

Magnetic Interaction Between Hard $SrFe_{12}O_{19}$-Soft $NiFe_2O_4$ Nanocomposite

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This work is to investigate the nature of magnetic interaction between $SrFe_{12}O_{19}$(hard) and soft ($NiFe_2O_4$) in a nanocomposite magnet. The sample 35% $SrFe_{12}O_{19}$+ 65% $NiFe_2O_4$ has been prepared by the one-pot sol gel auto-combustion method. The Rietveld refinement of XRD patterns confirms the existence of both hexagonal and cubic crystal symmetry. Both coercivity and saturation magnetization of the composite magnet is enhanced as compared to $NiFe_2O_4$. Hysteresis loops confirm single-step magnetization reversal of both soft and hard phases. The DC remanent magnetization and isothermal remanent magnetization measurements confirm the existence of interparticle interaction. The Henkel plot (δM vs H) has been utilized to study the nature of magnetic interaction. The dominance of exchange couple interaction has been observed over dipolar interaction. Magnetocrystalline anisotropy driven magnetic interaction has been analyzed by employing the Stoner-Wohlfarth model.

l) Energy materials

l0002

Ru Doped 2H/1T Multiphasic WS2 Nanosheets with Improved Supercapacitor Performance.

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The two dimensional layered transition metal dichalcogenides are well known supercapacitor electrode materials due to their structural, chemical, and physical properties. The transition metal doping is one possible pathway to enhance the active edge sites and charge transfer kinetics of these materials. In this study, we investigate the electrochemical supercapacitor performance of Ru doped WS2 nanosheets electrode. XRD and XPS studies have confirmed that Ru was successfully substituted into WS2 nanosheets and stabilized the 2H-hexagonal crystal phase up to 6at% of Ru in the samples. The higher Ru doping level (10 at%) results to possess 2H/1T multiphase WS2. The electrochemical supercapacitor measurement reveals that 2H/1T multiphasic WS2 sample exhibit improved specific capacitance (205 Fg^{-1} @ 0.5 Ag^{-1}) over the other samples in the 2H crystal phase.

l0003

Li-ion Conduction Mechanism and Its Pathways in Sorosilicate Compound $Li_2Cu_5Si_4O_{14}$

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Inorganic solid electrolytes are the building blocks for all-solid-state lithium-ion batteries. They have substantial advantages over organic liquid electrolytes i.e., enhanced safety and electrochemical properties, as well as mechanical stability. The present paper addresses the role of local crystal structure on the ionic conduction properties of a promising electrolyte material $Li_2Cu_5Si_4O_{14}$ by comprehensive impedance spectroscopy and neutron powder diffraction studies. The ionic conduction pathways within the unit cell have been mapped by the soft bond valence sum (BVS) analysis of measured neutron powder diffraction pattern. The analysis indicates the presence of bottlenecks in the lithium-ion conduction pathways along the a-axis as well as along the diagonal direction of the bc-plane of the triclinic unit cell. Such bottlenecks are responsible for the observed high value of activation energy, consequently, the moderate value of ionic conductivity. Understanding of microscopic conduction pathways will be helpful for designing efficient electrolyte materials.

l0004

Effect of Ca doping on resistivity and Seebeck coefficient in single crystal Bi_2Se_3

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A negative n-type Bi_2Se_3 crystal turns to p-type when suitably doped with Ca on Bi site. The thermoelectric properties of $Bi_{1-x}Ca_xSe_3$ (x = 0.005, 0.05) are very sensitive to doping concentration, electrical resistivity and Seebeck coefficient both decreases on increase in doping concentration x. The temperature-dependent resistivity is theoretically estimated within the framework of the electron-phonon scattering mechanism, the contribution to resistivity due to inherent low-frequency acoustic phonons characterized by Debye temperature (θ_D), as well high-frequency optical phonons characterized by Einstein temperature (θ_E) have been estimated. The thermoelectric power S(T) is estimated using phonon drag effect and is calculated within the relaxation time approximation. The anomalies reported in resistivity and Seebeck coefficient are successfully explained using the phonon scattering mechanism.

l0005

Analyzing Various Crystal Grains in the Multi-crystalline Silicon (mc-Si) Wafer for PV Applications

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We have studied the mc-Si wafers with different (hkl) planes. Initially, the wafer was chemically etched by KOH (20wt%) and IPA (2%) in the Millipore water at 60°C for 20 minutes. Now the various grains and their boundaries appeared clearly. Each grain has its own etch pit patterns and these are scanned by optical microscope. The area of each plane is measured by the Photoshop histogram tools with the input of a photographic image. The laser cut was made in various places (different etch patterns) to take the circular spot wafers for the X-ray diffraction measurement. The various (hkl) planes such as (111), (220), (311), (400), (331) and (442) appeared on the wafer. The optical reflectance studies reveal that the (400) plane has low reflectance and a high linear absorption coefficient compared to the other planes. Further, the resistivity of each (hkl) plane was measured by the four-probe method. It reveals that the (400) plane has minimum resistivity. <100> oriented grains are suitable for PV applications but the area of <100> is lesser than other grains like (111) and (442). The desired grain area can be increased using monocrystalline broken wafers as seeds and the orientation preselected should be favourable to enhance photovoltaic (PV) efficiency.

l0006

Ag and Se Double Substitution Leading to Enhanced Thermoelectric Performance in $Cu_{12}Sb_4S_{13}$ Tetrahderite

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The intrinsically low thermal conductivity in tetrahedrite ($Cu_{12}Sb_4S_{13}$) stems from the anisotropic vibration of the Cu 12e atom in the sulfur triangle. Ag substitution at Cu sites enhances the phonon scattering in the tetrahedrite unit cell and reduces the thermal conductivity. In this study, keeping Ag substitution the same, Se substitution for S 24g was varied for two samples. Se substitution increased the density of states effective mass (md*). So, the composition $Cu_{11.975}Ag_{0.025}Sb_4S_{12.7}Se_3$ had the highest Seebeck coefficient of 146.4 μV K^{-1} and a maximum power factor of 1.42 mW m^{-1} K^{-2}. Additionally, the analysis of the lattice part of thermal conductivity using the Callaway model indicated that the Se substitution could cause point defect scattering, and the lowest lattice part of thermal conductivity of ~ 0.36 W m^{-1} K^{-1} was obtained for the composition $Cu_{11.975}Ag_{0.025}Sb_4S_{12.8}Se_2$. As a result, the sample with the composition $Cu_{11.975}Ag_{0.025}Sb_4S_{12.7}Se_3$ exhibited a maximum value zT of 0.83 at 728 K. This work illustrates a successful method for simultaneously decoupling the adversely interdependent thermoelectric properties using isoelectric double substitution.

l0008

Substitution of Sn in Defective Half Heusler $Nb_{0.83}CoSb$ Under Different Sintering Conditions

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Defective 19 valence electron Half-Heusler ($Nb_{1-z}CoSb$) shows the short-range ordering of vacancy in the crystal structure, which gives a low electrical resistivity and thermal conductivity value. These intrinsic vacancies control the thermal conductivity and the concentration of charge carriers. The carrier concentration needs to be optimized for $Nb_{1-z}CoSb$, and there is still a chance to reduce lattice thermal conductivity. This work presents the thermoelectric properties of defective Half-Heusler by substituting Sn at the Sb site under different sintering conditions. $Nb_{0.80}CoSb$, $Nb_{0.83}CoSb_{1-x}Sn_x$ (x=0.00, 0.01, 0.03) are prepared by vacuum arc melting and vacuum hot press. Using the X-ray diffraction technique, the lattice parameter, strain, and crystalline size were calculated. The scanning electron microscope combined with the Energy dispersive X-ray spectroscopy (EDS) is used to measure the samples' composition. LSR-3 measured the electrical resistivity, Seebeck coefficient, and thermal diffusivity by LFA-1000 from RT to 980 K. The observed value of the Seebeck coefficient for the Nb0.80CoSb is -215.32 $\frac{\mu V}{K}$, and the zT value is 0.60 at 980 K.

l0009

The Synergetic Role of Bioactive Materials in Dye Sensitized Solar Cells for Lower Recombination and Higher Efficiency

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The current study investigates novel bioactive material-based co-sensitized Dye sensitized solar cells (DSSCs) as a potential approach of improving power conversion efficiency. To fabricate environmentally benign solar cells, red, orange, and pink Gerbera jamesonii flowers and Cajanus cajan leaves were co-sensitized (GRC, GOC and GPC) in 1:1 volume ratio. UV-Vis and FTIR spectra were used to examine the optical absorption and the presence of functional groups in the extracted dyes. The surface morphology of TiO2 film was examined through scanning electron microscopy (SEM). Electrochemical impedance spectroscopy and I-V characteristics analysis revealed GRC with maximum efficiency of 1.29% which was 1.25 and 2.08 times higher than GOC and GPC cells. This enhanced efficiency of GRC is higher than most of the earlier reported organic DSSCs.

l0010

Enhancing the Quality of mc-Si Ingot through Optimization of Partition Block in a DS System for Photovoltaic Applications

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The modified DS system has been constructed finite volume method using numerical simulation. A new partition block has been introduced at the side bottom of the crucible with dimensions of a length: 50 mm and a height: 110 mm, which relates to the existing portion block (dimension length: 50 and height 55 mm). This acts as a thermal partition block near the silica crucible bottom edge. The existing partition block system is considered a conventional system. The temperature distribution, power consumption, and thermal stress during the various solidification rates have been analyzed for both systems. In the modified case, power consumption minimizes and saved up to 1.5 kW/h, and flat or slightly convex m/c interfaces are achieved during solidification. The temperature gradient has been maintained properly in the modified case; hence the thermal stress of the grown mc-Si is lower than in the conventional case. Therefore, the better quality of the mc-Si ingot can be achieved through the modified DS furnace for Photovoltaic (PV) applications.

l0011

Experimental and Theoretical Investigations of Photocatalytic H_2 activity of 0D, 1D, and 2D CdS Nanostructures

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In recent years, we have witnessed a great deal of interest in semiconductor-based photocatalysts due to their potential to address major energy-related problems. Among these, Cadmium Sulfide (CdS) has turned into a well-known choice because of its exceptional photocatalytic properties and cost effectiveness. This work provides a comparison of the photocatalytic activity of CdS in 0D (microspheres), 1D (nanorods), and 2D (nanosheets) structure. Among the three, CdS nanorods exhibited high photocatalytic hydrogen evolution performance of about 2.5 mmol. g-1.h-1. which is nearly 2 and 1.3 times higher compared to 0D and 2D structure respectively. Also, the obtained band edge of each nanostructures lies around 520 to 550 nm emphasize their broad visible light absorption. Furthermore, the electronic structure and band alignment studies using density functional theory (DFT) found to be well in accordance with the experimental outcomes via proving 1D CdS hexagonal is more favorable for water redox reactions compared to cubic (0D) CdS nanostructures

l0012

Ag_3PO_4- Coconut Shell Derived Carbon composite for Visible Light Driven Photocatalysis

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Ag_3PO_4-coconut shell derived carbon (AgP-CSC) composites were successfully synthesized via a hydrothermal method. AgP-CSC composites with different weight percentages of coconut shell derived carbon (CSC) (1, 5, 10, 20 and 30 wt%) were developed. Composite sample with 10 wt% of CSC loading exhibits a high value of photodegradation coefficient under sunlight irradiation and this is about 42% higher than that with AgP only. The studies indicate that the approach is very simple and cost effective for developing visible light driven photocatalysts with superior catalytic activity.

l0013

Chemical Vapor Deposition of Two-Dimensional Semiconductor Heterojunction Solar Cells

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Atomically thin two-dimensional semiconductor nanolayers and heterostructures are the points of source for emerging exotic phenomena in materials technology. The direct bandgap of MoS_2 and WS_2 nanolayers makes them attractive for optoelectronic device application. Here, by employing the versatile chemical vapor deposition (CVD) technique, high quality TMDs semiconductor pn junctions such as MoS_2/WSe_2 and MoS_2/Ir-WS_2 (Ir doped WS_2) were deposited and reported their solar energy conversion property. Both MoS_2/WSe_2 and MoS_2/Ir-WS_2 heterostructures exhibit photovoltaic power conversion behavior under light illumination condition. The open circuit voltage (Voc) and short circuit current (Isc) are determined as 0.229 V and 0.339 μA for MoS_2/WSe_2, and 0.18V and 0.05μA for MoS_2/Ir-WS_2 device with power conversion efficiency less than 0.2% in both devices.

l0014

A Theoretical Study on Hydrogen Adsorption over Monolayer ZnO Substrate

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Adsorption of molecular hydrogen (H_2) over a hexagonal zinc oxide (ZnO) monolayer has been studied using a combined framework of van der Waals density functional theoretical (vdW-DFT) calculations and kinetic Monte-Carlo (kMC) simulation code. A landscape like adsorption energy profile has been depicted to understand the probability of adsorption of a single hydrogen molecule over different positions inside a hexagonal ring. The adsorption energy is found to be about 50 to 60 meV with a diffusion barrier of about 4 to 5 meV. The maximum number of hydrogen molecules to be adsorbed per hexagonal ring is three. The kMC simulation code indicates that a high amount of surface coverage of hydrogen molecules on ZnO substrate is possible at a few atmospheric pressure and temperature below 200 K.

l0015

Facile Synthesis of 3D Rice-Like BiOCl Nanostructure as a Negative Electrode Material for Supercapacitors Application

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3D porous rice-like BiOCl nanostructure was prepared via solvothermal technique with sodium chlorate as a surfactant which serve as negative electrode material for the supercapacitors application. The prepared nanoparticles supported on nickel foam textile exhibit high diffusion battery type charge storage in a 3 M KOH aqueous electrolyte solution. The dominance of the diffusion-type charge storage mechanism of the BiOCl electrode was confirmed through the CV study. Furthermore, the GCD study revealed a good specific capacitance with 213 F/g for 1 A/g current density and supports the application of BiOCl as negative electrode material for the supercapacitors.

l0016

Effects of Grain Size In Radiation-Induced Segregation Of Cr In Fe-Cr alloy

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Chromium-based ferritic steels are attracting considerable attention in the nuclear industry due to their microstructure and improved mechanical properties. In the present work, Fe-20%Cr samples have been irradiated with 225 keV Xe^+ ions at high temperature. Irradiation-induced segregation of Cr in Fe-Cr alloy is investigated in small (30 µm) and large (350 µm) grain size samples. Scanning Electron Microscopy (SEM) images show the Cr segregation at grain boundaries. High-Resolution Rutherford Backscattering (HRBS) measurements were carried out in the unirradiated and ion irradiated Fe-Cr samples. Our results reveal that, the Cr segregates at the projected range of the samples and the segregation is more pronounced in small-grain Fe-Cr sample

l0017

Exploring the Electrochemical Performance of Tunnel Structured $Na_{4.32}Mn_9O_{18}$ Cathode in Sodium-ion Coin Cell

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Sodium ion batteries are being considered as viable alternative to lithium ion batteries due to their low cost and abundant availability. Identifying earth-abundant, low-cost, and safe materials that can function as intercalation cathodes in Na-ion batteries is an important challenge facing the field. $Na_{4.32}Mn_9O_{18}$ exhibits reasonably high conductivity of 2.1×10^{-3} Smm^{-1} s^{-1} at 438 K, the mean temperature of measurement. Since high conductivity is a primary requisite for any material to be used as electrode in batteries, hence, the electrochemical performance of $Na_{4.32}Mn_9O_{18}$ has been explored when used as electrode in sodium ion battery (SIB). The tunnel structured $Na_{0.44}MnO_2$ is a well-researched cathode for SIBs with a theoretical capacity of ~ 122mAh g^{-1} within a voltage window of 2.0−4.0 V. The cycling performance of $Na_{4.32}Mn_9O_{18}$ at a current density of 0.05A g^{-1} and it delivers a discharge capacity of ~400.7 mAh g^{-1} even after a run of 3000 cycles. Incidentally, this is the first report on the electrochemical performance of tunnel structured $Na_{4.32}Mn_9O_{18}$ cathodes in sodium ion battery.

l0018

Enhanced Thermoelectric Properties of Cr doped BiCuSeO

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Oxychalcogenides have gained importance due to their properties, favorable for thermoelectric materials like: low thermal conductivity, thermal and chemical stability, tunable band structure, economical and environment friendly. Here we present the effect of Chromium doping in BiCuSeO. With a nominal amount of Cr doping the zT could be enhanced by ~185% from that of the parent compound (ie. from ~0.33 to 0.61) at 800K. The superior zT could be achieved due to the simultaneous enhancement of power factor and suppuration of thermal conductivity in the Cr doped sample.

l0019

MoS_2/BN/rGO Ternary Nanocomposite: A Visible - Light Driven Photocatalyst with Enhanced Photocatalytic Performance and Stability

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The present work is focused on the synthesis of 2D layered molybdenum disulfide/boron nitrate/reduced graphene oxide (MoS_2/BN/rGO) ternary nanocomposites were prepared for the first time through sonication assisted hydrothermal method. Flower, disk and layered morphology of MoS_2, BN and rGO, respectively was confirmed from field emission scanning electron microscopy (FESEM) images. Microstructural analysis was carried out using high resolution transmission electron microscopy (HRTEM) analysis. Optical property analysis were carried out using the UV-vis spectroscopy and photoluminescence. The

ternary nanocomposite revealed better degradation efficiency about 98% of degradation against methylene blue (MB) within 45 min and the recycle analysis revealed better stability for 7 cycles.

l0020

Device Structure Optimization of $Cs_2AgBiBr_6$-Based Perovskite Solar Cell Using SCAPS-1D

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Inorganic halide perovskite solar cells have attracted considerable interest due to their high efficiency and low fabrication cost. SCAPS-1D based design, simulation and optimization of perovskite solar cells using novel charge transport materials and perovskites have helped in the evaluation of efficiency and performance. Various parameters have an important impact on short circuit current density, open circuit voltage, fill factor and efficiency of the solar cell. This work modeled and analyzed perovskite solar cells based on $Cs_2AgBiBr_6$ with various electron transport layers and hole transport layers. SnO_2 as ETL and Cu_2O as HTL showed enhancement in the photo-conversion efficiency. The proposed device structure is FTO/SnO_2/$Cs_2AgBiBr_6$/Cu_2O/Ni. The optimized thickness of the perovskite layers was 800 nm. The enhanced PCE of 24.29% is obtained for our proposed structure

l0021

3D Printer Assisted Cotton Pappus Embedded Polymeric Nanocomposite Based Wearable and Sustainable Triboelectric Nanogenerator

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Herein, we have fabricated 3D printer assisted cotton pappus embedded CPD nanocomposite which is further used in designing of self-powered and wearable TENG (CPTNG). The reason behind the utilization of 3D printed mold is to enhance the output performance of the device by inducing more surface potential. Moreover, the high aspect ratio and presence of chemical groups of cotton pappus directly improves the output results of CPTNG device by generating more polarization. Thus, the fabricated self-powered and wearable CPTNG depicts outstanding output performance of 201V output voltage and 1.02W/m^2 power density under 12N axial pressure. Additionally, the environmental friendly and flexible properties of the device expand its utilization in the field of biomechanical energy harvester by harnessing the energy during wrist up-down and muscle movements and converting them into electrical energy. The energy conversion ability of the device has been monitored by lighting up 95 no of blue LEDs. Furthermore, the transmission of signal come out from finger bending movement is also monitored by using ARDUINO UNO setup. Thus, the CPTNG device may be helpful in future health monitoring unit.

l0022

Water Drop-mediated Triboelectric Nanogenerator Employing Microporous Polymeric Film, using Single-step Microwave Irradiation

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Over the years, significant efforts have been invested in harnessing water's energy for electricity generation. However, triboelectric nanogenerator (TENG) now offers a sustainable solution by converting the mechanical energy from water drops into electrical energy and thereby powering up small electronic devices. In this study, we report a contact electrification mediated, water drop-driven TENG using PDMS nanocomposite and silk as the two triboelectric layers. The polymeric nanocomposite was integrated with flower-like CuS nanoparticles and was uniquely fabricated through a single-step baking technique using microwave irradiation, resulting in the formation of micropores within the composite film. PTENG demonstrated an impressive voltage of 172 V and effectively illuminated 86 blue LEDs with a simple hand-imparted force. The exceptional sensitivity of 34.4 V/kPa allowed the device to efficiently harvest mechanical energy from water drops. Notably, when exposed to water splash from different heights, the PTENG produced varying output voltages that possibly make it suitable to be used as a velocity sensor and can harness energy from randomly falling raindrops.

l0023

Lithium enriched poly (ethylene oxide) / poly (methyl methacrylate) blend polymer based solid electrolyte films for solid state lithium battery applications

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Present work is centred around the investigations carried out on solid polymer electrolyte (SPE) films with prospective applications in all solid state batteries, developed using lithium nitrate ($LiNO_3$) enriched poly ethylene oxide (PEO) - poly methyl methacrylate (PMMA) polymer blend. These SPE films are prepared using solution casting method. Structural characterizations are carried out using XRD and FTIR techniques. Electrochemical impedance analysis is used to found out

ionic conductivity of the SPE films which is of the order of $1.34x10^{-5}$ Scm^{-1}. Lithium ion transport number is found to be 0.999 and cyclic voltammetry studies establish that the electrochemical stability window of the solid polymer electrolyte films is quite high and is around 5V.

l0025

Understanding the Activity of $Ni_xCu_{(1-x)}Co_2O_4$ Trimetallic Spinel Catalysts Towards Urea Oxidation Reaction

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Three catalysts NCC-1 ($Ni_{0.25}Cu_{0.75}Co_2O_4$), NCC-2 ($Ni_{0.50}Cu_{0.50}Co_2O_4$), and NCC-3 ($Ni_{0.75}Cu_{0.25}Co_2O_4$), were synthesized by the thermal decomposition of $Ni(NO_3)_2.6H_2O$, $Cu(NO_3)_2.6H_2O$ and $Co(NO_3)_2.6H_2O$ precursors. The prepared catalysts were subjected to different physical and electrochemical analyses including ICP-OES, XRD, SEM, HR-TEM, and CV analysis for urea oxidation reaction (UOR) application for energy conversion from waste. The enhanced UOR activity of the NCC-3 catalyst was attributed to the more Ni(III) active species well dispersed on a spinel matrix with longer crystallinity order.

l0027

Impedance Spectroscopy Study of Solid Electrolyte $Cu_2P_2O_7$

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The solid oxide fuel cell (SOFC) has attracted an attention as a potentially reliable, long-lasting, and affordable technology for producing electricity. Generally, SOFC operates at higher temperature (≥ 1000 °C) and significant efforts are given to lower the working temperature to reduce the operating cost. Here, we focus on a solid electrolyte material that can be operated at intermediate temperature (400 - 800 °C). We have investigated the oxygen ionic conductivity of $Cu_2P_2O_7$ by impedance spectroscopy. Oxygen ionic dc conductivity of $Cu_2P_2O_7$ has been determined to be 10^{-8} S cm^{-1} at 475 °C which increases with the increasing temperature and reaches to a value of 10^{-4} S cm^{-1} at 800 °C. The value of dc conductivity increases with temperature revealing the semiconductor like behavior of the studied compound. A possible correlated barrier hopping (CBH) mechanism for ionic transport is evident from the ac-conductivity study. Further, the modulus analysis suggests the conduction mechanism remains unchanged over the temperature range and relaxation process is found to be non-Debye type.

l0029

Effect of Mn and Ni doping and co-doping into $LiFePO_4$/C cathodes of Li ion batteries

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Mn and Ni doped and co-doped $LiFePO_4$/C composites were synthesized through solid state reaction. The structural characterizations of the as synthesized samples were done using X-ray diffraction and Fourier Transform Infrared Spectroscopy measurements. Electrochemical performance of the Mn and Ni doped and co-doped $LiFePO_4$/C composite electrodes were evaluated through cycle stability test and rate capability test. Theoretical insight into the effect of Mn and Ni doping and co-doping into olivine $LiFePO_4$ structure have also been obtained through Density Functional Theory and Nudged Elastic Band calculations and the theoretical results have been corroborated with experimental data.

l0031

Electrochemical Studies of BFO-BTO Nanocomposites at Room Temperature

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In this work, pure BFO and BFO-BTO nanocomposites are prepared using sol-gel auto combustion route in the empirical relation (1-x)BFO-(x)BTO where x=0.01, 0.03. The prepared nanostructures were studied for the changes in the structural, morphological and electrochemical studies due to composite formation at room temperature. The XRD analysis revealed the microstructural properties of the pure BFO and BFO-BTO nanocomposites. The size of the nanocomposites decreased to 57nm on increased BTO concentration. SEM images revealed agglomerated nanostructures which became more coagulated on increased BTO concentration that can be correlated to the microstrain from the XRD data. The specific capacitance was calculated from the CV graphs which showed decreased specific capacitance when compared to pure BFO. But, the specific capacitance values increased on increased molarity of the electrolyte. By further tuning the properties, these BFO-BTO nanostructures emerge as useful potential candidate for energy storage application.

l0032

Boosted Performance of Freestanding Binder-Free Supercapacitor Electrode by Functionalized MWCNT and Effectiveness in Electromagnetic Interference Shielding

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In materials science, chemical functionalization is a technique used to oxidize the surface of materials. Numerous researchers employ this method to enhance the interaction and dispersion of carbon nanotubes (CNTs). The most important factor in supercapacitors' adoption for industrial usage is their high specific capacitance. This study focuses on preparing the acid Functionalized MWCNT (FCNT) formed Bucky paper via the vacuum filtration method using commercially obtained MWCNTs procured from NANOCYL® NC7000^{TM} as precursors. Without damaging the MWCNT's tubular structures, the production and manufacture of supercapacitor electrodes using carboxylic acid functionalized multi-walled carbon nanotube (FCNT) have been reported in this study. Through treatment with an H_2SO4/HNO_3 combination, carboxylic functionalities were added to the surface of carbon nanotubes. These functionalized CNTs were used to create flexible freestanding binder-free supercapacitor electrodes with 5*5 cm^2 Bucky paper serving as current collectors. The structure of CNTs was maintained, according to experimental Raman spectroscopy data and XRD data, even after all oxidations. Fourier transform infrared spectroscopy was used to demonstrate the inclusion of functional groups. These characterizations showed an improved crystallinity and the presence of the residual functional group in the FCNT Bucky sheet. Using cyclic voltammetry (CV) and galvanostatic charge-discharge analysis, the electrodes' electrochemical characteristics were assessed. The galvanostatic charge/discharge curve showed that the pristine MWCNT has an improved specific capacitance from 61 to 153 F/g at a 0.5 A/g current density, after acid functionalization. FCNT has a tremendous and outperforming specific capacitance with good cycling stability (~96.4% after 10,000 cycles at 4 A g^{-1}). The fabricated MWCNT Bucky paper was also investigated for its EMI shielding ability. It was observed that the Bucky paper (Length=5 cm, Width=2.5 cm, and Thickness=148 µm) exhibited a total electromagnetic shielding efficiency (transmission coefficient) of 36 dB for the single layer and 48 dB for the double layer at 8.2. GHz to 12.4 GHz (X band) following transmission coefficient as a dominant shielding mechanism.

l0033

Performance of Heat Pipe with Nanorefrigerant at Different Inclination Angles

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In this study,aimed at improving the efficiency of the heat pipe with nanorefrigerant is presented. The effects of heat pipe, input power and angle of inclination were taken into consideration. The thermal resistance, thermal efficiency and temperature distribution in the evaporator area were evaluated. The experimental results clearly show thet heat pipe with nanorefrigerant as a working fluid, charge amount of 50%, tilt angle 900, input power 85W gives the highest efficiency and low thermal resistance. Increasing input power increases HP performance by approximately 47.4%.

l0034

Investigation of Modified Argon Gas Flow Tube Effects on Multi-Crystalline Silicon Ingot Growth Process For Solar Cell Application: Numerical Simulation

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Using the finite volume method, a directional solidification (DS) furnace used to grow a multi-crystalline silicon (mc-Si) ingot is numerically simulated in 2-dimensions. The impact of argon gas flow on the melt-free surface was studied using transient global simulations of oxygen and carbon-dependent transport in laboratory-scale DS furnaces for mc-Si ingots. Argon gas flow (AGF) over the melt-free surface affects the temperature of the upper part of the silicon melt. In the conventional furnace, AGF is opposite to the growth direction. In a modified furnace system, argon gas is distributed through the melt perpendicular to the growth direction. In the modified furnace, during the solidification process, the SiO evaporation flux at the top of the melt-free surface reduces, resulting in a decrease in oxygen concentration in the grown ingot. A modified AGF pattern that inhibits the reaction between SiO gas and hot graphite material shows an exponential reduction of carbon concentration in the as-grown ingot. The conventional ingot obtained the oxygen and carbon concentrations within 6.61E17 and 9.04E16 atoms/cm3 respectively and the modified ingot obtained the oxygen and carbon impurity concentrations within 2.2E17 and 5.32E16 atoms/cm3, respectively. The modified AGF tube improves the quality of mc-Si ingots for PV applications.

l0035

Supercapacitor applications of Cerium doped $BiVO_4$ nanosheets as electrode materials.

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Cerium doped 2D bismuth vanadate ($BiVO_4$) nanosheets were electrophoretically formed on Ni foam and used to make pseudocapacitor. Structural and electrochemical examinations were conducted in order to clarify the relationship between the physical characteristics of $BiVO_4$ and their capacity for charge storage. In this work we report successful preparation of cerium doped $BiVO_4$nanosheet and their electrochemical properties measured using cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS) and galvanostatic charge discharge (GCD). Structural factors confirmed by X-ray diffraction analysis (XRD) and morphological studies of the pure $BiVO_4$nanosheet confirmed by Scanning electron microscope (SEM) analysis. At a scan rate of 1 mVs^{-1}, cerium-doped $BiVO_4$ had a specific capacitance of 839.4 Fg^{-1} and a power density of 3.74 $kWkg^{-1}$.

l0036

Synthesis and characterization of Graphitic carbon nitride material used for comparative study towards electrochemical applications

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Carbon based Graphitic carbon nitride (g-CN) is synthesized via a single-step pyrolysis route using melamine as a precursor source. The X-ray diffraction analysis confirms the graphitic phase and FT-IR analysis reveals the layered structure of sp^2 hybridized C-N bonding features. The FESEM images observed irregular sheet like structure. The electrochemical performance of the g-CN electrode was investigated by cyclic voltammetry which exhibits good oxidation and reduction behavior, and these results are enhanced for future storage applications.

l0037

Correlation between the Structural, Vibrational and Electrochemical properties of $LiNiO_2$ and $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ cathode materials

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Layered structure $LiNiO_2$ and $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ are synthesized by sol-gel auto-combustion method at 900 ºC. The structural, vibrational and electrochemical properties of these cathode materials are investigated in detail. The XRD patterns of both the samples indexed to the α-$NaFeO_2$ layered structure with o detectable impurity phases. The Rietveld refinement was carried out which confirms the presence of rhombohedral symmetry with a space group of $R\bar{3}m$. The peaks of IR absorption bands for $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ powders are located at 509.20 and 603.71 cm^{-1}. In the electrochemical process, a little reduction in the materials initial capacity is compensated for by a considerable increase in cyclability. These findings support that one of the most appealing cathodes for real-world applications, particularly for high-rate lithium ion batteries used in electric vehicles.

l0038

Synthesis and characterization of tamarind seed husk derived carbon quantum dots incorporated polypyrrole nanocomposite for energy storage applications

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Recently, carbon quantum dots (CQDs) have become intensive research hotspots because of their unique characteristics such as small size, non-toxicity, high chemical stability, wide surface area, and high electrical conductivity. These properties are favorable for various potential applications. In this study, green synthesis of Tamarind Seed Husk derived carbon quantum dots (TCQDs) by a simple one step hydrothermal method, and Tamarind Seed Husk derived carbon quantum dots/Polypyrrole nanocomposites (TCQDs/PPy) was synthesized by using facile In-Situ chemical polymerization method. The synthesized TCQDs/PPy composite was characterized by using Fourier transform infrared spectrometer (FT-IR) to study the chemical interactions, and the morphological changes using a field emission microscope (FESEM) method. The optical properties were studied with the help of UV-Visible absorption spectroscopy, which shows $\pi \rightarrow \pi^*$ transition of C=C and $n \rightarrow \pi^*$ transition of C=O, which confirms the strong electron transition in the TCQDs/PPy composite. The electrochemical property of the TCQDs/PPy composite electrode were studied by cyclic voltammetry (CV) which signify the large surface area with a symmetric shape of the curve. These results suggest that the TCQDs/PPy composite electrode is a promising electrode for high energy storage applications.

l0039

Surface Modification of One-Step Facile Synthesis Ni_3S_2/MoS_2 Directly Grown On Ni-Foam as a Binder-Free Electrode for Ultra-High Supercapacitors

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Tuning the microstructure and composition of supercapacitor electrode materials is crucial for improving specific capacity, rate capability, and cycle stability. In this research article, we report the successful one-step hydrothermal synthesis of a surface-modified hierarchical Ni_3S_2/MoS_2 hybrid nanomaterial directly grown on Ni foam. The structural, morphological and electrochemical properties of the synthesized electrode materials were thoroughly analyzed. The as-synthesized Ni_3S_2/MoS_2 composite electrode exhibited an impressive specific capacity of 1387 F/g at 1 A/g and the electrode was stable in the electrochemical charge-discharge cycles desirable for supercapacitor applications.

l0040

Theoretical Investigations On Cobalt-Phosphorus Based Ternary Alloys For Energy Harvesting Applications.

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In this article, we investigated the study of XCoP (X = Ti, Zr, Hf) half-Heusler compounds within the density functional theory through full potential linearized augmented plane wave technique executed in WIEN2k. The investigated alloys are semiconductors with indirect band gap of s 1.36, 1.11 and 1.36 respectively. All the three reported alloys show ductile character with directional property and hence they are highly stable during experimental analysis. Transport properties have been computed at different temperatures by using semi-classical Boltzmann theory within constant relaxation time approximation. The calculated Seebeck coefficient of XCoP (X=Ti, Co, P) is 167 μV/K, 126 μV/K and 77 μV/K at 1200K. The compounds also exhibit good figure of merit at high temperatures. These compounds are suitable candidates for thermoelectric applications.

l0041

Li Ion Batteries with ZnO/TiO_2 Thin Film Anodes

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TiO_2/ZnOand ZnO/TiO_2thin film bi-layer electrodes have been deposited on polished stainless-steel (SS) and gold coated stainless-steel (SSG) substrates using rf and dc magnetron sputtering techniques. Li ion batteries (LIBs) have been prepared with these samples as anodes. During the cycling test, LIB with the ZnO/TiO_2/SSG electrode has marked a reversible capacity of 368 $mAhg^{-1}$ after 1000 cycles at $0.3Ag^{-1}$, exhibiting remarkable cyclic performance when compared to the LIB's other three bi-layer electrodes. To further increase the capacity and facilitate better capacity retention, we have divided a TiO_2/ZnO bi-layer into multiple thin bi-layer stacks of TiO_2/ZnO or in other words prepared TiO_2/ZnO multilayer electrodes. Furthermore, to tailor the effect of thickness, we have fabricated the multilayers with two thickness ratios of 1:1 (ML1) and 5:1 (ML2) of ZnO/TiO_2ineach nano bi-layer. During the cycling test, SSML1and SSGML2 have shown excellent specific capacities of 855 $mAhg^{-1}$and 899 $mAhg^{-1}$ respectively at current density of $0.3Ag^{-1}$even after 500 cycles of battery operation, revealing remarkable long-life performance. Moreover, reversible capacities of 631$mAhg^{-1}$and 477 $mAhg^{-1}$are still maintained for LIB's with SSGML2 and SSML1 electrodes respectively after 500 cycles at high current density of 3A g^{-1}.

l0042

FIRST-PRINCIPLES STUDY OF BISF MONOLAYERS IN ENERGY CONVERSION APPLICATIONS

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Highly efficient, environmental friendly and sustainable resources of energy are in great demand to overcome environmental pollution and the energy crisis. In this work, we have investigated the two-dimensional (2D) Janus BiSF monolayer using a first-principles approach and explored its potential applications in energy conversion fields, i.e., water splitting, solar cells, and thermoelectrics. The redox potentials of water are properly engulfed by the band alignment of the Janus BiSF monolayer. The calculated value of solar-to-hydrogen (STH) conversion efficiency of BiSF Janus monolayer is ~11%. We have also proposed heterojunction excitonic solar cells and demonstrated their power conversion efficiency (PCEs). Additionally, we have investigated the thermoelectric properties using semi-classical Boltzmann's transport theory. The appropriate value of power factor (PF) indicates that it can be a potential candidate for thermoelectric applications. Thus, our results affirm the potential applications of BiSF monolayers in energy conversion fields.

l0043

Rh decorated Cyclo[18]carbon: A Single-Atom Catalyst for Excellent Hydrogen Evolution Reaction

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In this study, we investigated the utilization of noble metal rhodium (Rh) on cyclo[18]carbon (C_{18}) as a single atom catalyst (SAC) for the purpose of enhancing the hydrogen evolution reaction (HER) activity using density functional theory (DFT). We analysed the geometry, stability, electronic properties and catalytic activity towards the HER of both C_{18} and Rh@C_{18}. The outcomes indicate a robust binding of the Rh atom to the support, evidenced by a notably high binding energy (E_b). The

calculated Gibbs free energy of hydrogen adsorption (ΔG_H) is -0.15 eV for $Rh@C_{18}$, which is in proximity to that of the best HER catalyst, such as Pt metal (-0.09 eV). Our findings strongly suggest that the engineered $Rh@C_{18}$ holds great promise as a highly stable and efficient SAC for HER activity.

l0044

Monocrystalline Silicon wafer recovery via chemical etching from end-of-life silicon solar panels for Solar cell Application

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Since more than 50 000 t of PV modules are anticipated to be worn out by 2025, the recycling strategy has been attracting a lot of interest in recent years. Metal electrodes, anti-reflection coatings, emitter layers, and p-n junctions must be eliminated from the solar cells in order to recover the Si wafers. In this study, we have carried out the etchant HF+ H2O2+ CH3COOH wet chemical etching methods to selectively recover Silicon wafers from end-of-life Silicon solar cell. A recovered Si wafer with a consistent and smooth surface was generated using this etching technique. The etched recycled wafers had characteristics that were nearly equal to those of commercial virgin wafers. The recycled silicon wafer's thickness was 250µm, resistivity was 1.6Ωcm, and minority carrier life time was 2.17µs, respectively. Additionally, the surface of recycled silicon wafers has an ultralow reflectivity of 12 % and commercial silicon wafers had reflectivity of 25%. The recycled wafer surface reflectivity was analysed by UV-Visible spectroscopy. The FTIR results indicate the reduction of oxidation in the etched samples (before etch and after etch). These characterizations helped us to understand the structure and properties of the end-of-life solar cell wafer.

l0045

Electrochemical performance of magnesium-doped $LiNi_{0.90}Mn_{0.05}Co_{0.05}O_2$ cathode material for lithium-ion batteries

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$LiNi_xMn_yCo_zO_2$ (NMC) cathodes in lithium-ion batteries (LIBs) are suitable for electric vehicle applications due to their competent balance of performance metrics. Each element in the NMC provides different properties with several drawbacks. Magnesium (Mg) doping in $LiNi_{0.90}Mn_{0.05}Co_{0.05}O_2$ (NMC-90) cathode minimizes those drawbacks, provides structural stability, avoids cation mixing, and offers reversible capacity. The co-precipitation technique is used in the synthesis of doped NMC cathodes. Here, the Rietveld refinement supports the identification of the phase and crystallinity of the material. Further, the single-crystalline nature of the Mg-doped NMC cathode is confirmed by FESEM. The co-precipitation synthesized in 1 mol% Mg-doped NMC-90 shows a better cation mixing level and retains a discharge capacity of 42% with 94% coulombic efficiency.

l0047

Surface Nitridated Silver Direct-Growth on Carbon Cloth for Active Hydrogen Evolution Reaction Catalyst

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Transition metal nitrides, carbides, and phosphides are well-known active catalysts for hydrogen evolution reaction (HER). Due to its semiconductive nature, attaining lowest overpotential with high stability, it has a tedious problem for practical applicability. HER reactions are occurring at the surface of the electrocatalyst. Nitrides in the bulk region of catalyst is the reason for lower electrical conductivity. Surface nitrides are the key factor for ameliorate HER. Silver is a well-known active catalyst for many applications. In this work, Ag is directly grown on carbon cloth, and its surface is nitridated to fabricate the active electrocatalyst. As-fabricated catalyst delivers ameliorated HER performance with Tafel slope of 322.77 mV dec^{-1}, overpotential of 101 mV at a current density of 10 mA cm^{-2}, and excellent stability.

l0048

Exploration of Lanthanum-based perovskites for pseudocapacitive electrode applications

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The scarcity of fossil fuels to promote sustainable energy storage development requires exploring highly efficient electrode materials. Lanthanum-based perovskites are regarded as an important perovskite in energy storage applications. A high-performance $LaBO_3$ (B=Mn, Fe, and Al) perovskite is synthesized using the sol-gel method as an electrode for supercapacitor applications. The structural conformation is done by XRD analysis, comparing it with JCPDS data of $LaBO_3$ (Mn, Fe, and Al). The electrochemical performance of all samples is done using cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS) in a 2 M KOH aqueous electrolyte solution. The $LaFeO_3$ electrode displays the highest specific capacity of 527 C g^{-1} at 1 A g^{-1} current density. It exhibits capacity retention of 46% and Coulombic efficiency of 99% after 5000 cycles at 10 A g^{-1}. The reported strategy facilitates the development of $LaFeO_3$ perovskites in electrode material as an energy storage application.

l0049

MXene/MWCNT Based Composite For Efficient Hydrogen Evolution Activity

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Hydrogen through water splitting has drawn a lot of interest as a result of the global energy crisis and environmental degradation. However, producing hydrogen for the longer period of time is still an important task. For achieving this, non-metal earth-abundant based electrocatalysts are required to replace the cost-effective catalysts like platinum. In recent developments have seen the adoption of two-dimensional (2D) transition metal carbides, nitrides are the potential candidate to replace the platinum based electrocatalyst as they better characteristics, including structural, good electrical conductivity and have high active surface area. Unfortunately, titanium carbide ($Ti_3C_2T_x$) based MXene have greater conductivity but shows very less stability in the environment. To overcome this issue composite having low dimensionality have better HER performance. In this present study, we outline the importance of MXene/MWCNT based composite approach for enhancing the HER properties. The MXene/MWCNT composite has lower overpotential of -0.18 V at current density of 10 mA/cm^2, and have a smaller Tafel slope of 132 mV/dec as compared with individual MXene and MWCNT. The catalyst also shows the good stability behavior after 3000 cycles. These all results suggests that the composite of MXene with MWCNT helps to replace the platinum based electrocatalysts.

l0051

Tris-(8-hydroxyquinoline)aluminium(Alq_3)/ZnO hybrid thin film based voltage controlled photodevice

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Abstract. Solution processed optoelectronic devices based on Zinc Oxide (ZnO) has gained extensive research importance in the recent years. Tris-(8-hydroxyquinoline)aluminium (Alq_3)/ZnO hybrid thin films were deposited using sol-gel derived spin coating method. UV visible spectra shows a higher transmittance (97% at 550 nm) and slight increase in the band gap of ZnO upon increasing Alq_3 content. PL studies show the decreased deep level/defect-related visible emission of ZnO in hybrid films, attributed to improved film quality due to the quantum confinement effect. Alq_3 incorporated ZnO films exhibit improved crystallinity evidenced by the increased peak intensity in XRD studies. UV light source assisted three-terminal photodevice to control the current upon applied voltage bias has been fabricated. The results showed that the photocurrent in the device is effectively controlled by the applied potential. The control-voltage induce the charge carriers into the ZnO or ZnO/Alq_3 films in the device and thus increase the photocurrent. A linear increase in photocurrent was observed to be increased for increasing applied bias voltage, making the device act as a constant resistance device. The study supports the incorporation of Alq_3 incorporated ZnO hybrid film will be very much useful for the application of photodetectors and phototransistors.

l0052

Microwave Assisted Mechanochemical Synthesis of $Na_{0.67}FeO_2$ as Cathode Material for Sodium-Ion Batteries

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Layered structured β-$Na_{0.67}FeO_2$ has been synthesized using mechanochemical method with microwave assisted heating. This modified approach of synthesis enabled formation of β-$Na_{0.67}FeO_2$ at much lower temperature (650 °C) and time (5h) than earlier reported. Structural characterization and phase identification was carried out using X-ray Diffraction (XRD) confirming the presence of desired phase with average crystallite size ($\bar{D}$) of 81 nm. Surface morphology and particle size were analyzed using Scanning Electron Microscope (SEM). Average particle size ($\bar{d}$) was calculated to be ~277 nm with particles having irregular spherical morphology. Specific surface area of these particles was found to be 2.83 m^{2}g^{-1} by BET method, with an average pore size of 36.88 nm

l0053

Exploring the Properties of Si-N Compounds as High Energy Density material: Using Density Functional Theory

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High-energy-density materials (HEDM) remains an active subject of investigation within the domains of materials science and industrial applications. Herein, we have explored silicon-nitrogen compounds with stoichiometries Si_3N_4 and SiN_2 using structure searching method combined with first-principles calculations. Among these, SiN_2 ($Pa\bar{3}$) is proposed as a HEDM with the energy density up to 1.88 kJ/gm. Amazingly, despite being subjected to lower synthetic pressure (~15 GPa) and having low nitrogen contents, this material exhibits a non-polymeric structure while maintaining energy density on par with various polymeric nitrides. An excellent explosive performance from the standpoint of higher detonation velocity (7.83 km/s) and detonation pressure (403.53 kbar) than that of TNT suggests SiN_2 as promising high-energy-density material candidate.

l0054

Improved Electrocatalytic Bifunctional Activity of Transition Metal Doped WS_2 Nanosheet.

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Two-dimensional layered transition metal dichalcogenides (TMDs) compounds (such as MoS_2 and WS_2) having a high density of exposed active sites show excellent electrochemical hydrogen evolution reaction (HER) activity but possess poor oxygen evolution reaction (OER) activity. Here, we report the improved electrochemical bifunctional activity of transition metal, Mn, Fe and Co, doped WS_2 nanosheets in 1M KOH electrolyte. It is observed that the cathode overpotential at a current density of 10 mA/cm^2 (η10) of the catalysts for HER has decreased in the order 403 > 372 > 282 > 130 mV for WS_2 > Mn-WS_2 > Fe-WS_2 > Co-WS_2 respectively. In addition, all catalysts also show OER activity simultaneously and produce anode onset potential (η_1@1mA/cm^2) in the order 1.91 > 1.84 > 1.76 >1.62 V for WS_2 > Mn-WS_2> Fe-WS_2 > Co-WS_2 respectively. Our study reveals that the simple doping strategy could help to improve the overall water-splitting bifunctional activity of TMDs nanostructures.

l0055

Microwave-assisted High Performance NiO Electrode With Short Reaction Time For Supercapacitor Applications

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Microwave-assisted method was used to prepare the nickel oxide (NiO) nanoparticles. XRD spectrum of NiO shows the cubic phase and good crystalline structure. The broad diffraction peaks exhibit the NiO nanoparticles having large surface area to volume ratio. FTIR spectroscopy reveals the functional groups present on the surface of NiO. NiO electrode improves the electrochemical properties of supercapacitor when the scan rate is increased from 5 mVs-1 to 80 mVs-1, and the area under the curve also increases. The Cyclic voltammetry (CV) curves are non-rectangular shape, attributed to the pseudocapacitive nature. The shape of the curves is nearly same even at higher scan rates, indicating the stability of the NiO electrode material. The high specific capacitance of 91 Fg-1 is obtained at 5 mVs-1 scan rate.

l0056

Structural and Thermoelectric Performance of $Bi_{2-x}Sb_xGeTe_4$

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Crystal structure, vibrational phonon modes and thermal transport property (*viz.* Seebeck coefficient) of Antimony (Sb) doped Bi_2GeTe_4 are investigated. Beside lattice strain and Stacking fault defect formation, crystallite size and lattice parameter (*a*, *c*) are also decreased owing to Sb substitution. An idea of compressive strain and phonon lifetime of the samples is acquired from Raman spectroscopic measurement. Remarkable enhancement (~135%) of Seebeck coefficient with Antimony (Sb) doping in Bi_2GeTe_4 is obtained. Minority carrier suppression is observed due to doping, which plays a positive role in improvement of TE performance.

l0057

Thermoelectric Transport Properties of Composites with MXene

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The research community is focused on creating renewable energy resources because of the growing human population's high energy needs and the scarcity of energy sources. The waste heat from thermal power plants, automobiles, and the steel industry can be converted into usable electricity via thermoelectric materials. However, the efficiency of a thermoelectric device has been a measure concern of the research community. Numerous strategies such as doping, nano-structuring, grain boundary engineering, and composite formation have been adopted to enhance thermoelectric response of the materials. Among those, compositing with a carbon-based material is a novel approach to enhance the transport properties of the material. In this research, we have studied the impact of composite formation on the thermoelectric properties of readily available thermoelectric materials. It has been shown how MXene incorporation affects the thermoelectric performance and power output values of the composite.

l0059

Rapid, Low-Temperature Synthesis of $Na_{0.67}CoO_2$ as Potential Cathode Material Application in Sodium-Ion Batteries

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Herein we report the synthesis of layer-structured P2-type $Na_{0.67}CoO_2$ using a facile mechanochemical approach assisted by microwave heating. This modification to the conventional synthesis route has enabled obtaining a pure phase material at a significantly lower temperature and time. Structural characterization via X-ray diffraction (XRD) reveals a P2-type phase, which is electrochemically favourable for cathode material application. The Scherrer formula applied to this data revealed an average crystallite size of 67.6 nm. SEM images show a polyhedral structure with stacking of plate-like morphology. Energy dispersive spectroscopy (EDS) on the powder sample indicates that the synthesized material matches the expected stoichiometry, $Na_{0.67}CoO_2$. The specific surface area of this compound was found to be 0.7 m^2g^{-1}, with an average pore size of 75.82 nm.

l0060

Na-ion Diffusion in Quaternary Chalcogenides, Na_3ZnGaX_4 (X=S, and Se)

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In this paper, we bring out atomic-level features of the diffusion process in these new materials Na3ZnGaX4 (X=S, Se) using quasielastic neutron scattering (QENS), and ab-initio molecular dynamics. The insights obtained from these techniques are unique and not available from other macroscopic experiments. Neutron scattering experiments have been performed at temperatures from 100 to 700 K. The simulations have been carried out up to 900 K. We have calculated the phonon spectra and the space-time correlation functions and found good agreement with the results of the neutron scattering experiments. The simulations enable detailed analysis of the atomic-site dependent dynamical information. We observe low-energy phonon modes of ~6 meV involving the vibrations of certain Na atoms in the lattice. This reveals that, among the two available crystallographic sites, the Na at 32g Wyckoff sites (Na2) has sufficiently shallow potential. This shallow potential facilitates diffusion. Furthermore,he specific structural topology of the network of interconnected zig-zag chains of the Na2 atomic sites provides the low-barrier energy pathways for diffusion. A small fraction of vacancy defects appears essential for diffusion. We further observe that the Na2 atoms undergo jump-like diffusion to the vacant next or the 2nd next neighbour sites at ~4 Å. While the QENS experiments reveal the jump-like diffusion and its time scale, detailed analysis of the AIMD simulations shows that the jumps appear mostly along zig-zag chains of the Na2 sites in the tetragonal ab-plane, as well as between the chains along the c-axis. The net diffusion is essentially 3-dimensional, with little anisotropy despite the anisotropy of the tetragonal crystal structure.

l0061

PVA-Gel Polymer Based Separator For Supercapacitors

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This work reports the comparison of polyvinyl alcohol-based gel electrolytes as compared to their aqueous counterparts. The prepared gel electrolyte was tested using reduced graphene oxide as the electrode material. The electrode material was characterized for structural and transport properties. A quasi-solid gel of Polyvinyl alcohol was dispersed in 1 M H2SO4 solution and used as an electrolyte. Symmetric supercapacitors were fabricated using the gel electrolyte as separator. The charge storage performance was studied using electrochemical techniques like cyclic voltammetry and galvanostatic charge-discharge. The electrochemical measurements confirm high gravimetric charge storage obtained for Gel based electrolyte of 48.4 F/g compared to aqueous based charge storage of 34.6 F/g at the current density of 1 A/g. The performance of the gel capacitor obtained was better compared to the traditional aqueous electrolyte-based capacitor. This device can be further studied for the flexibility of the device owing to its solid state nature of the electrolyte.

l0062

Effect of Precursor Concentration and Annealing Temperature on the Optical Properties of $Cs_2AgBiBr_6$ Perovskite Thin Film

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Perovskite materials have emerged as promising candidate for various optoelectronic applications due to their exceptional electronic, optical and catalytic properties. Recently, halide perovskite have attracted scientific attentions due to its excellent electronics and optical properties in optoelectronic applications. However, some major issues such as instability, toxicity and power conversion efficiency (PCE) need to be addressed before commercialization. In this work, $Cs_2AgBiBr_6$ lead-free double perovskite film is synthesized via single step spin coating method. We have investigated the effect of precursor solution and annealing temperature on the optical properties of the perovskite film. The UV-Vis analysis shows that the absorption of the film is influenced by the precursor concentration and annealing temperature. Further, the result indicates the influence of both the precursor concentration and annealing temperature on the band gap of the film. As the precursor concentration and annealing temperature the increases, the band gap of the film decreases. Hence, the study reveals that the annealing temperature and concentration of precursor plays an important role in the optical properties of the perovskite thin film.

l0063

Tin Rich SnS Electrode Material for Battery Type Supercapacitor Application

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This work illustrates the synthesis and fabrication of SnS electrode for energy storage application. A highly tin rich SnS nanomaterial was successfully synthesized by homogeneous precipitation technique. The crystalline phase of the nanomaterial was confirmed by X-Ray diffraction technique. Prepared SnS nanomaterial displays a higher specific capacity of 1675 C g^{-1} at the current density 1 A g^{-1}. The proposed nanomaterial possesses good rate performance of 1215 C g^{-1} at high current density of 5 A g^{-1}. It delivers an energy density of 67.5 Wh kg^{-1} at power density of 1200 W kg^{-1}. This metal chalcogenide enriched with metal ion allows an enhanced reversible electrochemical redox reaction that suitable for energy storage applications.

l0064

DFT and ML Coupled Halide Solid-State Electrolytes design for All-Solid-State Li-ion Batteries

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Lithium halide Li_3YCl_6, Li_3ErCl_6, Li_3InCl_6 are promising solid electrolyte (SE) candidates because of their outstanding electrochemical stability and superior ionic conductivity. In this work, we apply density functional theory (DFT) to investigate the impact of halide ions and their partial substitution with O and F atoms, on their thermodynamic, mechanical and transportation properties. Our result shows that Li_3YCl_6 and Li_3InCl_6 maintain their trigonal and monoclinic structures respectively, for up to 2.78 % O-substitution and 2.08 % F-substitution at Cl site. All these materials have energy above hull, $E_{hull} > 0$ eV/atom and are likely to be metastable. The monoclinic phases for Li_3InCl_6 and O doped compounds have smaller E_{hull} compared to the trigonal phases of O and F-substituted Li_3YCl_6 and Li_3ErCl_6 SEs. A "softer" mechanical nature for halide SEs is maintained for all the O substituted compounds. Regular increment of Li-ion conductivities is not observed for both O- and F-substituted Li_3YCl_6, Li_3ErCl_6 and Li_3InCl_6 at room temperature (RT). Machine learned interatomic potentials are employed to estimate the total energies of compounds and forces between atoms to explore new compounds. These results provide comprehensive insights into such halide compounds for their practical application as solid electrolytes.

l0065

Raman studies in (BixY1-x)2O3 (x = 0.2,0.4)

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Bi_2O_3 is known to undergo a structural phase transition from a monoclinic structure (α-Bi_2O_3) to a disordered-cubic (δ-Bi_2O_3) structure at 1003 K that possesses superionic oxygen conductivity. The superionic δ-Bi_2O_3 phase can be stabilised at ambient temperature by substitution of suitable rare-earth element as $(Bi_{1-x}RE_x)_2O_3$ (RE=Nd, Sm, Gd, Dy, Y). However, the role of crystal structure, host dynamics, and rare-earth (RE) substitutions in O-diffusion is yet not well understood. Here we present a comprehensive study of the structure and dynamics of Bi_2O_3 with different Y-doping concentrations ($(Bi_{1-x}Y_x)_2O_3$ (x=0, 0.2 and 0.4)) using Raman scattering experiments. Our Raman experiments show a significant change in the vibrational spectrum between normal α-Bi_2O_3 and superionic δ-Bi_2O_3 and a pronounced change with temperature in Y-doped compounds, revealing the presence of soft anharmonic phonons and the role of dynamics in fast oxygen diffusion.

l0066

Novel Thin Film Electrodes: Paving the Way for High-Capacity and Long-Lasting Li-Ion Batteries

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In this study, we have investigated Li-ion batteries (LIBs) with thin film electrodes for portable and miniaturized energy storage. Thin film electrodes of $LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$ (LNMC-333) and $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (LNMC-811) have been prepared using radio frequency magnetron sputtering technique on stainless-steel substrates. During cycling tests, LIBs with the Ni-rich LNMC-811 electrode exhibited high capacity but degraded quickly compared to LIBs with stoichiometric LNMC-333. To address this, a bi-layer structure has been fabricated with LNMC-333 as an outer (top) layer for stability and LNMC-811 as an inner (bottom) layer for high capacity. These bi-layer LIB's showed improved cyclability and stability over 100 cycles. We have subsequently developed a compact multilayer design with five bi-layers of LMNC-333/LNMC-811 and a concentration graded tri-layer structure of LMNC-333/LNMC-622/LNMC-811. Both structures demonstrated enhanced specific capacity compared to the bi-layer design, and the graded cathodes exhibited superior capacity retention over 500 cycles. Thus, the thin film route by magnetron sputtering technique used in this study offers a scalable and reproducible method for producing high specific capacity LIB's with stability, making it highly promising for micro battery applications.

l0067

Iron Oxide Modified Separator For Improved Performance In Lithium Sulfur Battery

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The capacity fading due to "polysulfide shuttling" is a major issue in Li-S batteries. In order to alleviate the issue, the separator has been modified by loading nano Fe_2O_3 via facile vacuum filtration route. The content of Fe_2O_3 has been varied systematically and the specific discharge capacities at varying current densities is evaluated. It is observed that at 100 mA/g, the cell utilizing 4mg iron oxide modified separator exhibits 480 mAh/g as compared to 364 mAh/g in case of pristine separator. The impedance of the cells also reduces and lithium diffusion coefficient increases nearly tenfold upon using the modified separator.

l0068

Enhanced Electrochemical Performance of Polyaniline-Coated Micron-Sized Sulfur Cathode for Lithium-Sulfur Batteries

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Li-S batteries have been strongly advocated as prominent alternatives to Li-ion batteries. The shuttling of lithium polysulfides (LiPS) during cycling is an intrinsic problem in Li-S batteries, resulting in significant capacity fading over cycling and impeding their practical applications. A simple yet effective method has been employed to synthesize polyaniline (PANI) coated sulfur particles that mitigate LiPS dissolution in the electrolyte. This study demonstrates a PANI-coated cathode with micron-sized sulfur particles (~7-9 µm) for high-performance Li-S batteries. This engineered cathode considerably alleviates rapid capacity fading, and the PANI coating effectively retains the LiPS within the cathode structure. The composite cathode exhibits an initial discharge capacity of 613 $mAhg^{-1}$ at a current density of 0.1 Ag^{-1}, retaining 98.7% of its capacity over 70 cycles.

l0069

Preparation of inorganic $AgBiI_4$ light absorbers for lead-free mesoscopic carbon-based solar cells

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Abstract. In recent years, organic-inorganic hybrid lead halide perovskite solar cells (PSCs) reached significant progress but they were made with harmful lead (Pb), which is one of the major obstacles to large-scale adoption. $AgBiI_4$ light absorbers have been identified as potentially lead-free and low-toxic materials for solar cell applications. $AgBiI_4$ was prepared by mixing AgI and BiI_3 precursors with a ratio of 1:1 M in DMSO: DMF solvents. A carbon-based inorganic lead-free Rudorffite ($AgBiI_4$) solar cell was fabricated under ambient conditions and observed 1.04 % of PCE under standard illumination test conditions.

l0070

Rationally Co-Sputtered Synthesized Pt-WO_3 @ SS Thin Film for High-Performance Super capacitive Application

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Abstract. In the present work, we have synthesized tungsten oxide and Platinum-tungsten oxide (Pt-WO_3) thin films using dc magnetron sputtering method on stainless steel substrate. After successfully deposition of thin film, the structural and compositional properties of thin film were investigated by X-ray diffraction (XRD), x-ray photoelectron spectroscopy (XPS) and energy dispersive X-ray spectroscopy (EDX). After that, we studied their electrochemical performance for supercapacitor application. These tests were done using cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS) and Galvanostatic charge-discharge techniques (GCD) in 1 M Na_2SO_4 aqueous electrolyte solution. The Pt insertion in WO_3 will improve its specific capacitance value from 225 Fg^{-1} to 550 Fg^{-1} at 0.1 $mAcm^{-2}$. Due to this high value of capacitance, Pt-WO_3 would be a potential candidate for supercapacitor device.

l0071

Insight Into Electrochemical Properties and Improved Performance of Manganese Iron Prussian Blue Analogue Cathode Material for Potassium Ion Battery

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Prussian blue (PB) and Mn doped PB (Mn-PB) thin films are electrochemically synthesized and investigated as cathode material of energy storage devices like batteries and supercapacitors. PB thin films are deposited on Pt electrode using a cycling voltammetry by varying the potential over -0.2 to 1 V in pH 2 solution containing 1mM FeCl3 and 1mM $K_3[Fe(CN)_6]$ compounds. Two pairs of intense peaks (Fe^{+3}/Fe^{+2}) are observed in PB thin film, manifested due to the redox reaction of hexacyanoferrate in 0.1 M KNO_3 electrolyte solution. The specific capacity and specific capacitance of PB film have been found to be 15 mC/cm^2 and ~10 mF/cm^2 at 10µA current. However, specific capacity and specific capacitance have been enhanced to 20 mC/cm^2 and 20 mF/cm2, respectively by optimizing the Mn doping in PB thin film. The presence of Mn provides an extra pair of redox peaks due to manganese hexacyanoferrate (Mn-HCF) which enables us to enhance discharge time of the electrode material. The electrochemical performance of the PB film has been significantly improved due to redox activity of Mn-HCF where films are found to be stable over 100 cycles at different current densities.

l0072

Exploring Zr-decorated Graphdiyne for Reversible Hydrogen Storage using Density Functional Theory

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Employing Using Density Functional Theory simulations, we investigate hydrogen storage in Zr-decorated Graphdiyne (GDY), an allotrope of carbon synthesised in 2010. Zr is tightly bonded to GDY, with a binding energy of -3.68eV on the hexagonal ring and -5.73 in the triangular ring due to charge transfer from Zr 4d-orbital to C 2p-orbital. A single GDY could store 4 Zr atoms, and each Zr atom could reversibly hold 7H2 molecules, with an average adsorption energy of -0.49eV and an average desorption temperature of -360.71 K, resulting in a gravimetric storage capacity of 8.35%, which is higher than the targets established by the US Department of Energy. Here, we have considered the hexagonal ring for trapping Zr since the triangular ring showed deformation on loading more H2 molecules, whereas the hexagonal ring decorated GDY remained sturdy. Kubas interaction, defined as charge donation from 1s orbitals of H to 4d orbital of Zr and a subsequent back donation, causes the strong binding of H2 to the GDY medium. The same is also verified using the Bader analysis. The stability of the medium is verified using AIMD and Phonopy simulations. Results suggest that Zr-decorated GDY can be an excellent storage system.

l0073
Characterization of Stable α-$FAPbI_3$ Microcrystals Synthesized via Retrograde Solubility-Driven Crystallization in an Ecofriendly Solvent
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Hybrid organic-inorganic halide perovskite-based semiconductor materials present formidable contenders to silicon-based materials. However, the growth of halide perovskite-based materials is hindered by long-term stability concerns associated with these perovskite materials. Formamidinium-based perovskites (e.g., FAPbI3) offer several advantages that make them promising materials for various optoelectronic applications. Herein, α-FAPbI3 microcrystals were synthesized by crystallization in green solvent. The synthesized α-FAPbI3 microcrystals are subjected to structural (XRD), optical (UV), morphological (FESEM), and compositional analysis (EDS). The XRD spectrum evidence the formation of the photoactive cubic phase FAPbI3. The wide absorption range and the energy band of the FAPbI3 microcrystals was examined by UV-Vis-NIR spectrum. The powder was also subjected to thermal (TGA), morphological (FESEM), and compositional analysis (EDS). Moreover, α-FAPbI3 microcrystals exhibit remarkable ambient stability, maintaining their properties for an impressive duration of 60 days without any observed phase transition.

l0074
$NiWO_4$-MCN Nanocomposite: Microwave-Assisted Synthesis and Superior Capacitive Behavior
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Electrochemical supercapacitors are pivotal in energy storage, with performance hinging on mechanisms like electrical double-layer capacitor (EDLC) and pseudocapacitance. This research explores the integration of $NiWO_4$ nanoparticles, synthesized via a microwave-assisted sol-gel process, with multiwall carbon nanotubes (MCN) to enhance these mechanisms. The resulting $NiWO_4$-MCN nanocomposite exhibited a specific capacitance of 270.3 F/g at 5 mV/s and 325 F/g at 1 A/g, demonstrating impressive stability with negligible capacitance loss over 3000 cycles. These findings spotlight the NiWO4 nanocomposite's potential in advanced energy storage applications.

l0075
Effects of Mechanical Hammering and Ball Milling on Cyclic Hydrogen Storage Behavior of Ti_2CrV Alloy
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The Ti_2CrV alloy buttons have been prepared by arc melting method and its cyclic stability for hydrogen absorption and desorption has been investigated for 50 cycles after mechanical hammering and ball milling. The sample showed a hydrogen storage capacity of 2.4 wt. % at room temperature and 20 bar pressure. As prepared Ti_2CrV alloy showed around 15% decrease in storage capacity up to 5th cycle whereas hammered and ball milled alloy showed 40% reduction in hydrogen storage capacity up to 8th cycle, and thereafter it remained un-altered up to 50th cycle. Observed variation in hydrogen storage capacity of the alloys has been attributed to the formation of thick oxide layer on alloy particles subjected to hammering and ball milling, as confirmed by energy dispersive X-ray analysis technique.

l0076
Thermoelectric Response of Graphene/ $Na_{0.75}CoO_2$ Thermocouple on Paper
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Flexible thermoelectric materials are presented with potential applications in electronic devices and energy conversion due to their convenient preparation, good flexibility and various forms. Here we report thermoelectric response of thermocouple device Graphene/$Na_{0.75}CoO_2$ based traces as “V” pattern draw on normal print paper. The output voltage of the

thermocouple device is 5.18 mV which is considerably good in comparison to other thermocouple devices. This convenient preparation method of these novel flexible thermoelectric materials may be expanded to the synthesis of other flexible thermoelectric materials, which will be the focus of future work.

l0078

Energy Storage and Water Splitting Performance of Microwave Synthesized $CuWO_4$/g-C_3N_4 Electrode Material

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This study reports a effective microwave synthesizing of CuWO4/g-C3N4 nanocomposites, and their potential as electrochemical supercapacitors and electrocatalysts for hydrogen and oxygen evolution reactions was completely examined. A specific capacitance of 111 F/g was detected in the study, indicating exceptional stability for supercapacitor applications. A remarkable bifunctional electrochemical performance can be observed by the nanocomposite, effectively permitting both HER and OER in different electrolytes. In particular, compared to bare CuWO4, it attained a conventional current density of 10 mA cm-2 with noticeably reduced overpotentials. These results emphasize the intriguing potential of CuWO4/g-C3N4 nanocomposites as versatile catalysts and energy storage materials.

l0079

Rapid Determination of Trace Uranium Concentrations in Ores and Minerals by INAA Method Utilizing Pneumatic Carrier Facility of Dhruva Reactor

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Rapid and nondestructive determination of trace quantities of Uranium in “as received” solid samples using a suitable analytical method is a challenging task. In the present work, Instrumental Neutron Activation Analysis (INAA) method has been optimized by standardizing sample mass, duration of irradiation, lesser decay period and faster counting to acquire reasonable counts (peak area) under the peak of interest. Pneumatic Carrier Facility (PCF) at Dhruva research reactor, has been advantageously utilized for short time irradiation (1 min) of the samples. The facility provides shooting of the sample into the core of the reactor for irradiation and receiving back the same to the laboratory pneumatically (via air pressure). Quantification of Uranium utilizing ^{239}U short-lived activation product (23.5 min half-life) formed after short irradiation, makes the methodology faster without any longer decay time. Uranium concentrations along with associated uncertainties and detection limits were calculated in ores and minerals having complex matrices like Zircon, Ilmenite and Rutile. The method was validated by analyzing USGS STM-1, RGM, AGV-1 and IAEA reference material RGU-1.

l0081

Au Enhanced Performance of CrN Symmetric Supercapacitor

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Recently, transition metal nitrides are being investigated extensively as potential supercapacitor material. In the present study, Au enhanced CrN thin films have been synthesized using reactive magnetron sputtering technique for application as supercapacitor electrode material. Electrochemical properties of the deposited material are investigated with a three-electrode system in 0.5 M H_2SO_4 as the aqueous electrolyte. The CrN thin film deposited under $8.75*10^{-3}$ mbar N2 partial pressure shows highest areal specific capacitance. As Au has been introduced, the film shows an aerial capacitance of 127 mF cm^{-2} at 1.0 mA cm^{-2} which is almost eight fold enhancement in specific capacitance value compared to pristine CrN sample. Furthermore, a symmetric supercapacitor have been developed which can deliver excellent specific capacitance of 110 mF cm-2 at 1.0 mA cm^{-2} with no decline in capacitance value till 20000 cycles. Results of the study clearly demonstrate these Au enhanced CrN films have great potential as energy storage material.

l0082

Exploration of Zircon to Host Eu^{3+} Phosphor Centre

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In order to explore the high temperature stable Zircon ($ZrSiO_4$) as host material for phosphor center, present work report the synthesis of $ZrSiO_4$:Eu via solid state route. The formation of Single phase $Zr_{1-x}Eu_xSiO_{4-\delta}$ (x= 0, 0.02) was confirmed through powder X-ray diffraction and FTIR spectroscopy. The emission profile of Eu^{3+} ion shows characteristic intra-4f transitions originating under D_{2d} local symmetry, which confirms the successful incorporation of aliovalent Eu^{3+} majorly at Zirconium site of $ZrSiO_4$ lattice. The corresponding excitation spectrum show intense O-Eu charge transfer band, indicating the significant transfer of energy from $ZrSiO_4$host to phosphor Eu^{3+} ion.

l0083

Effect of Surface Morphology of P3HT as a Hole Transporting Layer on the Photovoltaic Performance of Perovskite Solar Cells

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This study investigates the influence of surface morphology of poly(3-hexylthiophene) (P3HT) as a hole transporting layer on the photovoltaic performance of the perovskite solar cells. Varied morphologies are obtained through solvent processing, revealing a direct link between P3HT morphology and performance of perovskite solar cells (TiO2/MAPbI3/P3HT/Au). For this study, P3HT films were deposited from chloroform, dichlorobenzene, and their mixtures. The solar cells fabricated using P3HT film based on dichlorobenzene: chloroform (1:4) had the best photovoltaic performance, with a power conversion efficiency of ~17%. The cells were characterised by AFM, electrochemical frequency response analysis, and electroluminescent measurements. The study revealed that the better device performance of P3HT (dichlorobenzene: chloroform (1:4))-based cells was due to the low charge transfer resistance arising from the ordered structure of the P3HT films.

l0084

Optimization of Instrumental and Preconcentration NAA Methods for Rapid Determination of Selected Rare Earth Elements in Uranium-based Samples

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Rare earth elements (REEs) are extremely vital to modern technologies and society and are considered the most critical elements with applications in many areas like permanent magnets, sensors, light emitting diodes, batteries, magnetic resonance imaging (MRI) and catalysis. At the same time in nuclear industry, REEs like Dy, Eu, Sm and Gd having high neutron absorption cross section can act as neutron poisons and hence their accurate determination, along with other impurities, in uranium-based fuel is essential prior to their use in nuclear reactors. Instrumental Neutron Activation Analysis (INAA) method, in conjunction with short duration irradiation at PCF, Dhruva and faster counting, has been optimized with short-lived isotopes such as 161Gd, 165mDy and 153/155Sm for quantification of Gd, Dy and Sm respectively. Such isotopes are difficult to observe by conventional INAA with longer cooling periods owing to their very short half-lives (1 – 3 mins). It is also observed that 314.9 keV gamma (161Gd), 103.2 keV gammas (153Sm) and 108.2 keV gammas (165mDy) can be selected as characteristic gamma lines having remarkable figures of merit (FOM) due to their higher intensities.

l0085

Fabrication Of Carbon Based Mesoscopic Solar Cells Using Lead-Free Ag-Bi-I Light Absorbers

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Lead-free Ag-Bi-I Rudorffite materials, such as AgBiI4, Ag2BiI5, Ag3BiI6 and AgBi2I7 have gained significant attention as potential alternatives to lead halide perovskites for solar cell applications. However, most of Rudorffite solar cells are built with a mesoporous structure, which contains unstable and expensive hole transport layers (HTLs) along with noble metal electrodes. Herein, carbon-based Rudorffite solar cell is reported without expensive HTL and noble metal-electrode. Absorber layer of $AgBiI_4$, Ag_2BiI_5, Ag_3BiI_6 and $AgBi_2I_7$ materials synthesized through melt-solidification method. Under the ambient condition, $AgBiI_4$, Ag_2BiI_5, Ag_3BiI_6 and $AgBi_2I_7$ Rudorffite solar cells are fabricated. Among these fabricated solar cells, Ag_2BiI_5solar cells have high efficiency of 0.93% with an open-circuit voltage (VOC) of 0.707 V and short-circuit current density (JSC) of 3.09 mA/cm^2.

l0086

Calorimetric Investigation of ternary oxides in the CuO-V2O5 system

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Present study investigates the thermodynamic properties of ternary copper vanadate compounds, namely, CuV2O6(s), Cu2V2O7(s), Cu3V2O8(s), Cu5V2O10(s) and Cu11V6O26(s). A high temperature calorimeter was employed for measuring the enthalpy of dissolution of Cu-V-O compounds in sodium molybdate solvent (3Na2O:4MoO3). From enthalpy of dissolution data, standard molar enthalpy of formation of these ternary oxides was determined. The values of standard molar enthalpies of formation were found to be -1750.05 ± 3.03, -1948.77 ± 3.95, -2142.53 ± 5.37, -2507.46 ± 7.83 and -6770.54 ± 15.68 kJ mol-1, respectively for CuV2O6(s), Cu2V2O7(s), Cu3V2O8(s), Cu5V2O10(s) and Cu11V6O26(s). These experimental results coupled with the literature data were employed for generating thermodynamic functions and hence, predicting the thermodynamic stability of these compounds.

l0087

Exploring Penta-SiP_2 Monolayer For Overall Photocatalytic Water Splitting

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Low-dimensional materials have attracted enormously towards photocatalytic water splitting (PWS). Here, we studied the structural, electronic, and the photocatalytic properties of penta-SiP_2 monolayer using first principle calculations. It is observed to have an indirect nature with a band gap of 1.88 and 2.71 eV calculated using PBE and HSE06 functional, respectively. The valence band maximum is positioned close to X-point and the conduction band minimum lies along the M-Γ direction. The electronic band gap falls in the visible energy region and the band edge alignments with respect to vacuum straddles across both the redox potentials. The calculated HER Gibbs free energy (ΔG) under zero external potential (U_e) is 1.25 eV, indicating inertness of the catalyst. Further, under the effect of U_e, the ΔG reduces to 0.42 eV. The *OOH intermediate breaks on adsorption indicating that OER cannot proceed further. This implies that penta-SiP_2 remains inert to overall PWS though ΔG for HER enhances under the effect of applied external potential. We believe that our study will help researchers in understanding and designing of pentagonal structures as catalysts for photocatalysis.

l0088

Thermodynamic Characterization of NaMnF3(s) and Na_3VF_6(s) Compounds

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In the study, thermodynamic stability of NaMnF3(s) and Na3VF6(s) compounds has been investigated which can be formed due to interaction of structural components manganese and vanadium with secondary coolant salt (FLiNaK) of Molten salt reactor (MSR). An isoperibol solution calorimeter, maintained at 298.15 K was used to determine the standard molar enthalpy of formation ($\Delta_f H_m^\circ$) of NaMnF3(s) and Na3VF6(s) employing 150 mL of 3 M HCl solution as calorimetric solvent. The $\Delta_f H_m^\circ$ values of NaMnF3(s) and Na3VF6(s) compounds were found to be -1424.06 ± 1.08 and -3000.97 ± 2.29 kJ mol-1, respectively. These experimental results coupled with the literature data will be employed for generating thermodynamic functions. These functions will be useful for predicting the thermodynamic stability, possibility of formation and the behaviour of these compounds under reactor operation conditions.

l0089

Investigation of Local Structure and Co Vacancy in TiCoSb1+x: XANES And EXAFS Studies

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$TiCoSb_{1+x}$ (x=0, 0.01, 0.02, 0.03, 0.04, 0.06) mid-temperature thermoelectric (TE) maters are synthesized by solid state reaction method. Presence of defects and disorder in the $TiCoSb_{1+x}$ HH alloys are investigated employing X-ray absorption spectroscopy (XAS) studies. In order to carry out XAS studies, absorption data are taken at Co K-edge in transmission mode. Experiments are performed at BL-9 beamline, INDUS-2 synchrotron source (2.5 GeV, 200 mA), Raja Ramanna Centre for Advanced Technology (RRCAT), Indore, India. The Co K-edge spectrums are the result of excitation of electrons from 1s to the unoccupied 4p level, final state. Evidence of Co-vacancy in the $TiCoSb_{1+x}$ HH alloy is successfully revealed from analysis of XAS data. Change in Local structural parameters around Co in $TiCoSb_{1+x}$ samples are reported in the article. Increase in Sb concentration in $TiCoSb_{1+x}$ causes decrease in 1st and 2nd shell volume owing to the existence of Co vacancy in synthesized samples. However, the crystalline order in the short range is mainly preserved due to the negligible change in 2nd shell (Co-Sb) for the TiCoSb samples.

l0090

Combustion-assisted Nanocarbon Particles For Supercapacitor Application

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The application of carbon nanoparticles is ever-gaining attention in energy storage devices because of their physico-chemical properties influenced by surface morphology, surface area, porosity, and surface-active groups. This work aims at the synthesis of carbon nanoparticles obtained from the thermal combustion of Neem seed oil using a simple in-house built novel oil-lamp setup. Scanning electron microscopy (SEM) and X-ray diffraction studies have confirmed the amorphous nature of spherically shaped particles of about 40nm. BET surface area of grown carbon particles is found to be 100 m^2/g. Electrochemical characterization was carried out using cyclic voltammetry and galvanostatic charge-discharge studies of a two-electrode symmetric cell comprising polymer binder-carbon composite electrodes separated by electrolyte membrane soaked in 1M Na_2SO_4 solution. The initial studies have indicated that carbon nanoparticles thus obtained can be potentially applied as electrodes for Electrolytic Double Layer Capacitor (EDLC) applications.

l0091

Microstructural and Ionic Transport Studies of Sonochemically Synthesized Lead (II) Fluoride

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All solid-state fluoride ion batteries (FIB) are promising energy storage systems because of their high energy density. In this work, the classical superionic conductor Lead Fluoride (PbF_2) is prepared by the sonochemical method, and its microstructural aspects and ionic conductivity are investigated. Fine powders of PbF_2 are synthesized utilizing two different power levels of the ultrasonic probe, leading to different particle sizes and surface morphology. The crystallographic structure, surface morphology, and electrical properties of the sample are investigated to identify it as prominent anode material. A facile sonication process is employed to synthesize composite material comprising PbF_2 wrapped with Reduced Graphene Oxide (rGO). The ionic conductivity of the PbF_2/rGO is investigated through the impedance spectroscopy technique to understand the ion transport mechanism. The studies have demonstrated the possibility of PbF_2/rGO composite as a promising anode material for FIBs.

l0092

Nickel Diselenide (NiSe2) for Dual-Functional Applications as Symmetric Supercapacitor and Photocatalyst Dye Degradation

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In this study, $NiSe_2$ have been prepared via a hydrothermal route. The formation of the as-prepared sample is confirmed through X-ray diffraction (XRD) and field emission scanning electron microscope (FESEM) coupled with energy-dispersive spectroscope (EDS). Electrochemical testing of the formed $NiSe_2$ for a symmetric supercapacitor cell shows a specific capacitance (Csp) of 250 F g^{-1} @ 10 mV s^{-1}. It exhibits an energy density (Ed) of 21.7 Wh Kg^{-1} @ power density (Pd) of 800 W Kg^{-1}. The photocatalytic performance of $NiSe_2$ is examined by the degradation of Methyl Orange (MO). The $NiSe_2$ exhibits superior catalytic performance with a 92% elimination efficiency for MO after 80 minutes irradiation under sunlight. The results show that $NiSe_2$ is an effective dual-functional material for energy storage and photocatalytic applications.

l0093

Pseudocapacitive Kinetics in Reactively Sputtered Titanium Nitride Nanopyramids for High-Performance Flexible Supercapacitive Electrode

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The present study reports a flexible supercapacitor electrode of Titanium nitride (TiN) nanopyramids reactively sputtered over stainless-steel mesh (SSM) substrates via DC magnetron sputtering. The TiN/SSM electrode manifests fast pseudocapacitive kinetics in 1 M Na_2SO_4 electrolyte, thus delivering a high areal (25.53 mF.cm^{-2}) and gravimetric (212.73 F.g^{-1}) capacitance at 0.075 mA.cm^{-2}. Over a 100-fold increase in current density (0.075 mA.cm^{-2} to 7.5 mA.cm^{-2}), TiN/SSM displays an excellent 59.29% rate capability, thus illustrating the TiN/SSM electrode applicability in high-current device applications. In addition, the TiN/SSM flexible electrode delivers an impressive energy density of 4.26 μWh.cm^{-2} (25.83 Wh.kg^{-1}) and a high power density of 3.0 mW.cm^{-2} (25.0 kW.kg^{-1}). Further, the TiN/SSM flexible electrode exhibits nearly no deterioration, retaining 99.28% capacitance and 99.03% coulombic efficiency in the long-term cycling performance over 5000 GCD cycles at 2.0 mA.cm^{-2}. This is the standard font and layout for the individual paragraphs.

l0094

ZnO Buffer Layer Induced Improvement in the Photovoltaic Performance of Nitrogen Doped ZnO-Silicon Heterostructure

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ZnO is an ideal semiconductor buffer layer for perovskite, CdTe thin films and Si heterojunction solar cells. Here, we report the improvement in the solar cell performance of nitrogen doped ZnO-Si heterojunction (*p*-N-ZnO/*n*-ZnO/*n*-Si) having undoped ZnO buffer layer. In this work, N-ZnO thin film with *p*-type conductivity (E_g=3 eV) is used as a hole transport layer in *n*-type Si substrate. The solar cell made with *p*-N-ZnO/*n*-Si exhibits 0.080V open circuit voltage. The introduction of ZnO buffer layer in the heterostructure (*p*-ZnO/*n*-ZnO/*n*-Si) enhanced the V_{oc} (0.284 V) and conversion efficiency. Further, the solar cell numerical simulations on *p*-ZnO/*n*-ZnO/*n*-Si heterostructure have shed light on unraveling the mechanism of charge transport in the solar cell.

l0095

Temperature-dependent photoluminescence studies of guanidinium cation incorporate methyl ammonium lead iodide perovskite

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Organometal halides perovskites have received much attention in optoelectronic devices due to their high absorption coefficient, long diffusion length, and cost-effectiveness [1, 2]. In this work, we have studied the temperature-dependent photoluminescence (PL) properties for methyl ammonium lead iodide perovskite ($MAPbI_3$) and Guanidinium doped

MAPbI3 ($MA_{1-x}Gua_xPbI_3$ (X=5%)) under the excitation of 580 nm over a range of 80 K to 300 K as shown in the figure. We have observed discontinuities in the PL wavelength shift as a function of temperature as reported by Milot et.al [3] which arises due to the different band overlaps of two different phases (Orthorhombic, Tetragonal). The incorporation of cation (Gua) into ($MAPbI_3$), leads to increase the band gap due to higher ionic radius of Gua (278pm) than MA(217pm). The increase in the band gap of $MA_{1-x}Gua_xPbI_3$ causes the blue shift in PL intensity [4]. Furthermore, we have estimated the optical phonon energy of 28.17 meV and 28.01 meV for $MAPbI_3$ and $MA_{1-x}Gua_xPbI_3$, respectively, indicating the presence of exciton-phonon interaction in both samples. These outcomes provide essential insights into the optical properties of these hybrid perovskites, thus encouraging future applications in optoelectronics.

l0096

Consequence of the degeneracy of partially filled d-orbitals dopant in Cu_2CoSnS_4 thin film absorbing layer for Solar cell application

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The fabrication of polycrystalline Cu_2CoSnS_4 and Fe-doped Cu_2CoSnS_4 thin film by thermal evaporation method. From XRD the higher angle shift in diffraction peaks indicates the incorporation of the dopant Fe in the CCTS. The increase in band gap and shift in Fermi level indicates the CCTS underwent Burstein Moss effect. From the Mott Schottky plot indicates the reduction in valance band edge which in turn increased the band gap and decreased the Urbach energy there by increasing photo conversion efficiency of the photoelectrochemical cell.

l0097

One-step synthesis of α-Fe_2O_3 microcrystals and their superior PEC performance for water splitting

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This paper gives insights into the structure and PEC performance of densely grown, intimately connected, and highly [$2\bar{1}0$] oriented microcrystals (MCs) of hematite, used as a photoanode for water splitting. The MCs were grown on low-cost pure Fe substrates by simple and one step thermal oxidation method. XRD and XPS measurements carried out before and after PEC measurement confirms excellent stability of the photoanode in alkaline electrochemical environment. XPS measurements show that Fe is in +3 oxidation state. FESEM measurement reveals that these microcrystals are intimately connected and grow vertically on the Fe substrate. TEM measurement confirms single crystalline nature of the individual microcrystals (MCs). Linear Scale voltammetry (LSV) measurement shows photocurrent density of 0.14 mA/cm^2 at an applied bias of 1.23 V_{RHE} under chopped light illumination. Mott-Schottky measurement reveals n-type semiconducting nature of the MCs with donor density of 4.45×10^{18} cm^{-3} and flat band potential at -0.06 V_{RHE}. These results endorse the suitability of the hematite MCs as a promising candidate for PEC water splitting.

l0098

High Power Factor due in Ni doped in TiCoSb Half-Heusler Alloy

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Structural and transport properties of $TiCo_{1-x}Ni_xSb$ HH alloy is studied. TiCo1-xNixSb (x=0, 0.01, 0.02, 0.03, 0.04, 0.06) Half-Heusler polycrystalline samples were synthesized by solid state reaction method followed by arc melting of constituent elements. X-ray diffraction (XRD) measurements were carried out to analyze the phase purity and structural perfection of the samples. Successful replacement of Ni at Co site is observed from the Rietveld refinement. Further, mix-phase Rietveld refinement reveled presence of small amount of CoTi embedded phases in the $TiCo_{1-x}Ni_xSb$ matrix. Williamson-Hall plots indicate an improvement of structural order as Ni concentration increases from x=0 to x=0.02 owing to the decreases of CoTi embedded phases in $TiCo_{1-x}Ni_xSb$ matrix. Thermoelectric property is enhanced for $TiCo_{0.98}Ni_{0.02}Sb$. Resistivity decreases with Ni concentration owing to an increases in carrier concentration. However, thermopower increases with Ni concentration for $0\leq x\leq0.02$, owing to the change from multi-band conduction to single-band conduction. A further increase in Ni concentration ($0.02<x\leq0.06$) decreases S due to the increase in carrier concentration. As a result of the simultaneous increase in S and σ, an increase in PF of about ~250% is reported for $TiCo_{0.98}Ni_{0.02}Sb$.

l0099

Nanoscale Dielectric Capacitor using T-graphene.

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In this work, using density functional theory, the possibility of a T-graphene based nanoscale dielectric capacitor (NDC) with T-graphene like BN sheet as the dielectric material has been investigated. From band structure analysis on BN-doped T-

graphene, an indirect band gap of 4.08 eV is observed. This T-graphene like BN sheet has been introduced between parallelly placed T-graphene layers and the NDC obtained is tested. External voltages ranging from 0-1 V has been applied across the NDC for getting the Mulliken charge profile as well as the induced charge vs bias voltage which gives us the capacitance of the system. The slope of the induced charge *vs.* bias voltage indicates a capacitance of 9.35 Farad/gram for the NDC.

l0100

Tailored Antisolvent Engineering on $CsPbI_3$ Perovskite for Black Phase Stabilization at Low Temperature

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Inorganic perovskites ($CsPbI_3$) emerge as an attractive alternative to the hybrid organic-inorganic perovskites because of their potential for enduring high thermal stress. Despite being a thermally stable perovskite structure at elevated temperature (>310°C), $CsPbI_3$ also offer a suitable optical bandgap which makes it an ideal candidate for high-performance perovskite/silicon tandem solar cell architecture. Irrespective of the high efficiency for regular $CsPbI_3$ solar cells, the poor stability for adverse dopants reflects the importance of an inverted architecture. For feasible integration in the tandem geometry, it becomes a challenge to fabricate $CsPbI_3$ in the inverted (p-i-n) geometry at low temperatures. Here, we report the use of dilute additive engineering with DMAI and different antisolvent engineering (ethyl acetate, toluene, anisole and chlorobenzene) to tailor and stabilize $CsPbI_3$ films at a lower processing temperature of 100°C. As a result, well-oriented orthorhombic γ–phase is obtained with a more compact crystal lattice volume. Besides, the phase stability and robustness against external erosions also get a considerable promotion. Importantly, the inorganic-rich film still retain the black phase under a relative humidity of 65±2% under ambient air conditions. This work thus provides an alternative and simple way to tailor the $CsPbI_3$ perovskite films suitable for high efficiency inverted solar cells suitable for tandem geometry.

l0101

Carbon Dioxide Reduction over Single Atom (Co) Catalyst (g-C_3N_4): A Reaction Mechanism Study

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Exploration of two dimensional material with multifunctional properties have led to the investigation of recently developed single atom catalyst (SAC), a material with dispersed metal atoms across the surface of catalyst. Here, we studied electronic and optical properties of Co-g-C_3N_4 SAC which shows wide band gap with intermediate band as deep trap site. N-Co pπ-dπ interaction facilitating charge conjugation across the surface for high intermediate absorptivity which is an intrinsic property seen for Co-g-C_3N_4 SAC. CO_2 reduction reaction with probable reaction intermediates and possible reaction pathways have been optimized over the surface using an ab-initio study on Co-g-C_3N_4 SAC. Co site shows CO_2 physisorption with *C formation showing highest adsorption energy difference, while N site involve formation of *CH_2OH, which is considered as the reaction intermediate for most feasible pathway of CO_2RR over Co-g-C_3N_4 SAC. The ease of CO_2 adsorption, feasible reaction pathway, high visible light absorbance, and low adsorption energy difference makes it a potential candidate for high photo-conversion efficiency and as a suitable photocatalyst for carbon dioxide reduction reaction.

l0102

Exploring Temperature Dependent Synthesis of SnS_2 Nanosheets for Enhanced PEC Properties

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In this study, we have synthesized SnS_2 nanosheets using the hydrothermal method at two distinct temperatures, 130 °C and 180 °C. The electrical, optical, and photoelectrochemical properties are explored to understand the impact of temperature during synthesis. The process yields uniform nanosheets of SnS_2 when grown at 180 °C (referred to as SnS_2-180), while non-uniform growth of SnS_2, comprising irregular nanosheets and nanoparticles, occurs at 130 °C (referred to as SnS_2-130). The prepared samples of SnS_2 are used as photoanodes for photoelectrochemical (PEC) measurements. The SnS_2-180 nanosheets-based photoanode exhibits excellent photocurrent density (0.36 mA/cm^2), whereas the SnS_2-130 photoanode showed a lower photocurrent density (0.02 mA/cm^2) at 0.8V versus Ag/AgCl reference electrode. Collectively, these results highlight the potential of the SnS_2 nanosheets for PEC water-splitting applications.

l0103

Synthesis of Undulated ZnO Nanostructure and Its Effect as an Electron Transporting Layer on the Photovoltaic Performance of inverted polymer Solar Cells

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Undulated ZnO has recently showed the potential as an electron transport layer in polymer solar cells. The synthesis of these undulated ZnO structures has predominantly been achieved through sol-gel methods using ramp annealing method. However, the annealing temperature is around 200 ^{0}C, which is not suitable for fabrication of flexible polymer solar cells because of instability of their substrates at that temperature. Here, we show an alternative approach for synthesizing undulated ZnO using sol- gel method at 150 ^{0}C by varying the concentration of precursor solution. This study not only optimizes the precursor

concentration necessary for achieving the desired undulated structure but also demonstrates the manipulation of the undulation's height and length. The undulated ZnO was used as an electron transporting layer in inverted polymer solar cell exhibiting efficiency above 10% out performing ZnO nanoparticle based solar cells.

l0104

Effect of architecture of mesoporous silica incorporated TiO_2 photoelectrode on the performance of Dye-Sensitized Solar Cells

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In this paper, we have investigated the effect of architecture of mesoporous silica (m-SiO_2) incorporated TiO_2 photoelectrode on the power conversion efficiency of Dye-sensitized solar cell (DSSC). We found that m-SiO_2 had optimum effect when used in single layer approach with an improvement of 30% in comparison to double layer approach. This is mainly due to the uniform distribution of m-SiO_2 in TiO_2 photoelectrode and absence of an interface between two layers as is present in double layer approach, which in turn leads to the loss of charge carriers at the interface.

l0106

Effect of In doping and Embedded Phases on structural and Thermoelectric properties of SnTe

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$Sn_{1-x}In_xTe$ (x=0.00, 0.02, 0.04, and 0.05) samples are synthesized by solid state reaction method. Effect on structural, resistivity (ρ) and thermopower (S) for In doping in SnTe thermoelectric (TE) material are reported. X-ray diffraction (XRD) and in-depth structural analysis, employing Reitveld refinement confirm the incorporation of In in the position of Sn. Minute amount of embedded phases are obtained in the host matrix from Reitveld analysis. Dislocation density and strain are estimated from XRD data. In doping and embedded phases cause a resonance level and shift in Fermi surface in the host matrix. $Sn_{0.96}In_{0.04}Te$ that 4% In doped sample shows maximum S and correspondingly maximum host phases amid the In doped SnTe samples. Highest power factor is obtained for $Sn_{0.96}In_{0.04}Te$ synthesized sample. Room temperature structural and transport properties are corroborated in this endeavor.

m) 1-D, 2-D and quantum material

m0001

Piezoresistive Pressure Sensors and Wearable Strain Sensors Using van der Waals V_2O_5 Films

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Pressure sensors find various applications in the field of medical equipment, industries, scientific instruments etc. They employ different materials exhibiting piezoresistive/piezoelectric behavior, such as lead zirconate titanate (PZT), polyvinylidene fluoride (PVDF), ZnO etc. either in bulk or in thin film form. Recently, two-dimensional (2D) materials are reported to be suitable candidates for use in such piezoresistive sensors. 2D materials have strong intralayer bonding between atoms with only weak van der Waals interaction between the layers. Owing to the atomically thin nature, 2D layers show high susceptibility to external pressure, causing deformation in the nanosheets and the ensuing change in their bandstructure. This leads to change in resistance, and hence allowing them to exhibit piezoresistivity and making suitable for pressure sensing. While there are many reports on piezoressitive property and pressure sensing of grapheme, grapheme oxide (GO), reduced grapheme oxide (RGO), MoS_2 etc., there are negligible studies on vanadium oxides. Especially, to our knowledge, there are no reports on the piezoresistive property of vanadium pentoxide (V_2O_5) which is a van der Waals interaction based layered material. In this study, we have shown that drop cast films of V_2O_5 show excellent piezoresistive property when used for pressure sensing applications. Wearable strain sensors for detecting physiological movements of a human being, such as, figure bending, blinking of eye and swallowing were also demonstrated using V_2O_5 films.

m0002

Defect Studies in $MoSe_{1.8}S_{0.2}$ Using Resonant Raman Spectroscopy

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Using resonant Raman spectroscopy with 632.8nm (1.96 eV) laser, we describe the Raman spectra of single crystals of $MoSe_{(2-x)}S_x$ with a nominal composition of x=0.2. A few wavenumber difference in prominent Raman mode frequencies at various regions of the sample indicated Se deficiency. At low temperatures around 77K, we observed unusual temperature dependent enhancement in the intensity of non-zone centre modes as well as overtones and combination modes in Raman spectra. This enhancement in the intensity can be correlated to the resonance being achieved in the non-stoichiometric regions of $MoSe_{1.8}S_{0.2}$, at low temperatures when the defect level matches with the excitation energy.

m0003

Hydrothermally Synthesized Luminescent Carbon Quantum Dots from Cow Milk and Their Optical Properties

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Abstract. The hydrothermal process was used to synthesize carbon quantum dots (CQDs) from cow milk. The method employed is easy, one-step, and environmentally friendly. CQDs are approximately spherical in shape, having a typical size of 8 nm. They exhibited intriguing features such as a wide excitation and emission band, excitation-dependent emission, temperature-dependent photoluminescence behavior, the presence of diverse functional groups, and remarkable photostability with storage duration, UV irradiation, and high salt conditions. They have uses in cell imaging, ion sensing, photocatalysis, and optoelectronics.

m0004

Microwave-Assisted Synthesis of Bismuth Cupper Oxytelluride for Optoelectronic and Photodetection Applications

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Abstract. Over the last few years, quaternary-based bismuth copper oxychalcogenide BiCuOCh (Ch = S, Se, and Te) materials have caught much attention due to their exciting optoelectronic, thermo-electric, and semiconducting applications. Most of the studies on this 2D material are based only on thermoelectric properties or first principle calculations and much attention has not been given to explore other potential characteristics of this material. In this work, we have synthesized BiCuOTe using the facile "Microwave (MW) assisted method," which is not yet reported for preparing this material. The crystallographic studies are in good accordance with the previously reported phases and nanosheet-like morphology was observed. The band gap observed using diffuse reflectance spectroscopy (DRS) technique for this material is 2.04 eV, and the broad photoluminescence emission spectrum shows the suitability of this material for various optoelectronic applications. Results from the photo-response study suggest the potential applicability of this material as a photodetector.

m0005

Effect of Defects To Tailor The Structural and Electronic Properties of Zigzag GaN Nanoribbons

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Abstract. Defects are an integral part of any nanomaterial under pragmatic conditions. The presence of defects can significantly affect the electronic properties of nanomaterials under consideration. Therefore, in the present manuscript, we investigate the effect of vacancy and Stone-Wales defects (SWD) on the structural and electronic properties of zigzag GaN nanoribbons (ZGaNNR). It is revealed that the incorporation of considered defects is an exothermic process and the proposed structures are energetically feasible to be obtained. Furthermore, the electronic properties of ZGaNNR are highly influenced via incorporation of vacancy or SWD. A semiconductor to metallic transition for the vacancy defects whereas reduction in the band gap has been witnessed for SWD. Our findings indicate that apart from tailoring the electronic properties, these defects can also be used to induce n-type or p-type doping character in the material.

m0006
Synthesis and Investigation of Optical Properties of Amino Functionalized Graphene Quantum Dots Thin Film
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Abstract. This study includes the synthesis and investigation of optical properties of nitrogen-doped graphene quantum dots thin film on quartz substrate prepared using hydrothermal and spin-coating method. The XRD results had confirmed the hexagonal honeycomb structure of prepared sample. The average crystallite size calculated using Debye-Scherrer's formula has been found to be 2.879 nm. Further, the UV - Visible study shows a high absorption peak at 361 nm with direct band gap of 2.67 eV calculated using Tauc's plot. It was observed that prepared thin film shows high optical transmittance of 87% in the visible region. In addition to this, the PL emission spectrum has been studied at different excitation wavelength of 325 nm, 340 nm, 360 nm and 380 nm which indicate the high luminescent properties of thin film in the visible region. It was found that the emission intensity had increased with the increase in excitation wavelength up to 380 nm which shows its applicability in the photo luminescent devices.

m0007
Ab-Initio Study of 1T-NiX_2 (X=S, Se) Monolayers for Optoelectronic Applications
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Abstract. In this study, ab-initio calculations are employed for investigating the structural and optoelectronic characteristics of 1T-NiX_2 (X = S, Se) monolayers. It is observed that with an increase in chalcogen atom size, the lattice constant increases and the band gap decreases. The structural and dynamical stability of NiX_2 monolayers are confirmed by their negative cohesive energy and lack of negative frequency in the phonon dispersion spectra. With absorption coefficients reaching maximum values of 5 x 10^5 cm^{-1} for 1T-NiS_2 and 4.67 x 10^5 cm^{-1} for 1T-$NiSe_2$, both monolayers show great potential for applications in optoelectronic devices.

m0008
Inelastic Neutron Scattering Study of Trimmer Ruthenate, $Ba_5Ru_3O_{12}$
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We report the detailed Inelastic Neutron Scattering (INS) measurement of the $Ba_5Ru_3O_{12}$ system which undergoes long-range antiferromagnetic ordering at T_N =60K. In this system θ_{CW} is negative (θ_{CW}= -118K), indicating dominant AFM interaction, and is higher than T_N, which suggests magnetic frustration. For $Ba_5Ru_3O_{12}$, there are three Ru_3O_{12}-trimers which are isolated and has three distinct Ru with three different Wyckoff positions. This is distinct from other similar trimer systems, like $Ba_4Ru_3O_{10}$, $BaRuO_3$, $Ba_5LnRu_3O_{12}$, etc. We have performed the INS with E_i= 11meV, 30meV and 60meV at various temperature from 2-300K. We observe two strong magnetic excitation below T_N at ~ 5 meV and 10 meV. Interestingly, this excitation does not completely vanish even at very high temperature above T_N which suggest presence of short-range magnetic correlation in this trimmer system. Our INS elucidate the magnetic ground state of this unique system.

m0009
Structural, Magnetic and Magneto-Transport Properties of Single Crystalline $Fe_{3-x}GeTe_2$
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Investigations of structural, magnetic, electrical transport and magneto-transport studies of single crystalline $Fe_{3-x}GeTe_2$ have been reported. Single crystal of $Fe_{3-x}GeTe_2$ crystallizing in hexagonal structure is two-dimensional van der Waals bonded layered material in nature. Temperature dependence of dc magnetic susceptibility of the grown crystal confirms paramagnetic

to ferromagnetic long range magnetic ordering at ~180 K. Temperature and magnetic field dependent magnetization reveal magnetic anisotropy, crystallographic c-axis being the easy magnetization direction. Effective magnetic moment is found to be ~3.76 μB/Fe and the calculated large positive paramagnetic Curie temperature indicates the dominant ferromagnetic interaction in $Fe_{3-x}GeTe_2$. Magnetization vs. magnetic field at 5 K shows saturation of magnetization with a value 1.39 μ_B/Fe. The occurrence of an additional anomaly in the temperature dependent dc magnetization in different fields may hint for another magnetic ordering or spin reorientation transition or spin texturing behavior as the features of a skyrmionic material. Electrical and magneto-transport measurements reveal a magnon dominated scattering mechanism in $Fe_{3-x}GeTe_2$.

m0010

Structural and Physical Properties of disordered Kagome Lattice $Ho_3Sb_3Zn_2O_{14}$

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Studying physical properties along with crystal and magnetic structure is a promising way to perceive intriguing physics behind entangled quantum states $RE_3Sb_3A_2O_{14}$ class of compounds, which are mainly derived from pyrochlore structures ($A_2B_2O_7$) structures, known as Kagome compounds. These are corner sharing triangular lattice structures. In pyrochlore lattices A_3B and B_3A layers are stacked alternatively with non-magnetic ions giving an isolated two-dimensional Kagome lattice. Due to its triangular geometry, Kagome lattice exhibits geometric frustration. In the Tripod Kagome Lattice (TKL) compound, spins remain entangled and do not order in the zero-temperature limit. Therefore, they prove to be potential candidates for Quantum Spin Liquid (QSL). Here, we report synthesis, structural and magnetic properties of one of the Kagome lattice-based compounds with RE = Ho and A = Zn. X-ray diffraction, neutron diffraction, magnetization and specific heat have been employed to characterize structural and magnetic properties. Through analysis of structural data, we have observed disorder in the compound, and magnetic and specific heat characterizations suggests absence of long-range ordering down to 3 K.

m0011

Effect of Surface Engineering on 2D MXene using Heteroatoms and Terminal Groups

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Abstract. $Ti_3C_2T_x$ gets attached to other materials and alternatively stacked to form a layered composite through hydrogen bonding or electrostatic force. As the surface-active functional groups are anions, this makes the $Ti_3C_2T_x$ electronegative and prone to cations resulting in proper intercalation. Thus, the surface-decorated terminal groups present in $Ti_3C_2T_x$ help the substances to adhere to the base layers properly.

m0012

Raman Scattering Study of Cd_3As_2

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Abstract. Single crystals of Cd_3As_2 has been grown and characterized by Raman scattering measurements. Low frequency Raman spectra give some weak phonon peaks whose temperature dependence shows an intricate interplay of phonon and electronic degrees of freedom. The lower frequency phonons are related to the vibration of Cd ions, hence the anomalous anharmonicities in the Raman shift and width of these phonons are result of their coupling to Dirac states close to the Fermi energy. This behavior is governed by a characteristic temperature T^*~ 100K which is related to the mutual fluctuations of lattice and electronic degrees of freedom.

m0013

First-Principles Study of Be-Based Two-Dimensional Materials and Their Commensurate Heterostructure

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Abstract. Density functional theory has been employed to assess the electronic and mechanical properties of two-dimensional (2D) experimentally realized BeO and BeN_4 monolayers exhibit insulating and Dirac semi-metallic nature, respectively. The mechanical properties of monolayer BeO and BeN_4 indicate their isotropic and anisotropic natures, respectively. In addition, we also developed a novel commensurate semimetal-semiconductor van der Waals Heterostructure (vdWH) combining BeN_4 and experimentally realized MoO_3 monolayer. The calculated electronic band structure of BeN_4/ MoO_3 heterostructure clearly illustrates the ohmic contact of bands without employing any sort of fields that is useful for the high performance of devices. Hence BeN_4/MoO_3 heterostructure appears to be an appealing choice for use in applications involving nanoscale devices and energy storage.

m0014

An *ab-initio* Study on metal-WS_2 Interface

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Schottky and tunnel barrier formation at the interface of metal and semiconductor impedes the charge carrier transport in 2D materials-based electronic devices. Using an *ab-initio* model, we have investigated the interface between a monolayer WS_2 (a semiconductor) and a metal (e.g., Pd) to determine the Schottky and tunnel barriers. Through the effective potential calculations, the tunnel barrier height was found to be 7.95 eV. The Schottky barrier height was computed using the electronic band structure and density of states and found to be 0.66 eV. A Fermi-level shift was observed in WS_2 due to the interaction of Pd suggesting that WS_2 act as an *n*-type semiconductor with palladium contacts. Our calculations demonstrate that with the optimized separation distance of 2.14 A^0 there is an orbital overlap between metal and semiconductor.

m0016

Doping of Sn Atoms on WS_2 Surface: LEED and First Principles Study

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Abstract. We report here experimental and first principle theoretical studies on substitutional doping of Sn at the top S sites of the mechanically cleaved WS_2 surface under UHV conditions. Our in-situ low energy electron diffraction (LEED) measurements on both bare WS_2 and after Sn deposition indicates hexagonal symmetry of the surface, which is further validated by density functional theory (DFT) calculations. The calculated band structure of the Sn doped WS_2 surface reveals a metallic nature and the density of states calculations show electronic states constituted by hybridized states of W *d* and Sn *p* orbitals.

m0017

Experimental and Theoretical Understanding of Magnetization Plateau in Frustrated S=1/2 Antiferromagnetic Trimerized Heisenberg Spin Chain

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Quantum magnetization plateaus in low-dimensional spin systems have garnered a great deal of attention and have been investigated extensively in recent years. In this work, we have investigated the S = 1/2 Heisenberg antiferromagnetic $J_1 - J_1 - J_2$ trimerized spin chain with frustration through next-nearest-neighbour interaction J_3 in the presence of the magnetic field, where J is the antiferromagnetic exchange interaction constant. The presence of 1/3 magnetization plateau in ground state magnetization is studied for the ratios $\alpha = 0.18$, $\beta = 0.18$, and $J_1 = 235$K for relatively large lattice size N = 402, where $\alpha = J_2/J_1$, and $\beta = J_3/J_1$. It is found that the 1/3 magnetization plateau retains at very low temperatures and it gradually declines at temperatures higher than 45 K due to thermal fluctuations. Further, Isothermal magnetization results are compared with its experimental realization in $Na_2Cu_3Ge_4O_{12}$.

m0018

Effect of Thermal Annealing on Structural And Optical Properties of MoS_2 Quantum Dots Decorated Graphene Oxide Thin Film

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Graphene based nanomaterials have attracted considerable attention due to their unique optical and electrical properties. In this work, the impact of thermal annealing at different temperatures on Graphene Oxide (GO) sheets decorated with Molybdenum Disulfide Quantum Dots (MoS_2 QDs) was studied. The thin film was prepared by integrating MoS_2 QDs on the surface of large area GO sheets deposited using Langmuir-Blodgett technique, creating a hybrid material with enhanced properties. To examine the influence of annealing, samples were subjected to different temperatures in a controlled environment. The outcome shows that annealing at different temperature leads to significant modifications in the structural and optical properties of GO-MoS_2 QD. TEM measurement shows the homogenous spreading of MoS_2 QDs on GO sheets. The Raman and FTIR spectra associated with GO-MOS_2 QD annealed at different temperature shows the alteration in the lattice structure and chemical bonding. The insights gained from this study holds significant implication for designing and optimizing GO sheets decorated with MoS_2 QD for applications in batteries, supercapacitors and optoelectronic devices.

m0019

Investigating the Fano-Asymmetry Parameter in hBN Nanosheets Annealed at Various Temperatures

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Hexagonal boron nitride (hBN) nanosheets have been synthesized by a liquid phase exfoliation method followed by post-synthesis annealing treatments in hydrogen gas medium at various temperatures. A systematic effect due to temperature variation is observed in the morphological, vibrational, and structural properties of hBN. When the temperature treatment is applied up to 800°C, it has declined the crystallinity of hBN as observed from the broadening of XRD peaks. However, treating it above 800°C has improved the crystallinity of hBNNS. Raman spectra analysis also reveals some critical parameters along with the broadening of a peak, such as the Fano asymmetry parameter (q) has also been observed. The increasing asymmetry

(low q value) is observed while treating hBNNS up to 800°C, whereas the peak shows high symmetry (high q value) when treated at 1000°C. Scanning electron microscopy (SEM) has confirmed the presence of hBN nanosheets on Si substrate. The quality of hBN nanosheets has not significantly affected by lower-temperature heat treatment. The heat treatment at 1000°C has improved the quality of nanosheets.

m0020

Magnetic Properties of Two-Dimensional Distorted Triangular Lattice system $Na_3Fe(PO_4)_2$: A Neutron Diffraction Investigation

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Abstract. We present a comprehensive investigation of low temperature magnetic properties of two-dimensional (2D) layered geometrically frustrated triangular lattice spin-5/2 system $Na_3Fe(PO_4)_2$. The compound $Na_3Fe(PO_4)_2$ is constituted with the magnetic triangular lattice having two different NN exchange interactions J_1 and J_2. The bulk magnetization results reveal long-range AFM ordering below ~10.8 K. The analysis of low temperature neutron diffraction data reveals a commensurate (CM) collinear AFM spin structure. Such a collinear magnetic state is unique as compared to the in-plane 120° AFM structure reported for a regular and isotropic triangular lattice antiferromagnetic system. The present study provides an in-depth knowledge of magnetic ground state and its underlying origin in-terms of lattice distortions in the triangular lattice.

m0022

Investigation of Spin-correlations of Single-chain Magnet, $Sr_4Mn_2CoO_9$, through Neutron Diffraction

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Abstract: We present a comprehensive investigation of the magnetic structure and spin-spin correlations in $Sr_4Mn_2CoO_9$, revealing intricate dynamics of its structural and magnetic arrangements. This compound shows single-chain magnetic behavior with huge frequency dependence from 8 to 15 K for frequency range 10 Hz to 104 Hz.,[1] followed by single chain magnetic (SCM) behavior at low T below ~15K. We have performed neutron diffraction (ND) in detail. The (Co^{2+} - Mn^{4+} - Mn^{4+}) unit adopts a (↑↓↑) spin-state configuration along the chains, arranged on a triangular lattice, associated with k= (000) wave vector. We speculate that exchange-striction within each chain breaks the spatial inversion symmetry which leads to the generation of polarization. These findings shed light on the multiferroic effect in the system and contribute to a deeper understanding of the intriguing interplay between magnetic properties and lattice dynamics.

m0023

Study of Structural, Optical and Electronic Properties of Ni doped CdS Quantum Dot

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Abstract:
Colloidal Quantum Dots (QDs) have gaining significant research interest for application in optoelectronic devices. In this work, pure and Ni doped CdS Quantum Dots (QDs) were synthesized via chemical route. The X-ray data reveal that pure and Ni doped CdS QDs exhibit zinc blend structure with no trace of phase impurity. The particle size is ~2 nm confirmed by XRD analysis. Raman analysis reveals that intensity of longitudinal optical (LO) mode decreases with Ni doping due to short range structural disorder. Optical absorption spectra reveal that band gap energy decreases with increase in Ni concentration. Green luminescence under UV light has been observed from room temperature photoluminescence. X-ray photoelectron spectroscopy (XPS) study reveals the presence of Ni ion.

m0024

Role of Scattering Mechanisms in the Anomalous Hall Effect of two-dimensional Ferromagnet Fe_3GeTe_2

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Two-dimensional (2D) materials have attracted immense attention in the field of spintronics and electronic devices due to their novel spin dependent transport properties and the feasibility of fabricating complex structures out of them. Fe_3GeTe_2 (FGT) is a two-dimensional van der Waals bonded layered compound that shows high-temperature itinerant ferromagnetism. It has gained notable interest due to its attractive properties like uniaxial magnetocrystalline anisotropy, Kondo lattice behavior , planar topological Hall effect and ionic gate tunable room temperature ferromagnetism. Being an itinerant ferromagnet with high T_c and a candidate of nodal line semimetal, FGT has been the best platform to study the interrelation between ferromagnetism and topology. Here, we study the aspects of the scattering mechanism in the single crystal of high-T_c Fe_3GeTe_2 via magnetotransport and Hall effect measurements. Our results provide a clear understanding of the role of electron-magnon scattering on the temperature-driven evolution of the anomalous Hall effect that rules out its origin to be the topological band structure [1].

m0025

Magnetic Properties of Quasi-1D Vanadate NiV_2O_6

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Quasi one-dimensional Nickel vanadate, NiV_2O_6, was investigated using dc-magnetization, ac-susceptibility and heat capacity measurements as function of temperature and magnetic field. The compound crystallizes in triclinic structure with $P\bar{1}$ space group. The dc magnetization, ac-susceptibility and specific heat data indicate antiferromagnetic transition at ~15.6 K. Further, the magnetic behavior of this compound seems to change in low temperature region of 4 K to 13 K as indicated by several experimental signatures in magnetization and heat capacity data, and these changes are sensitive to magnetic field. Magnetic isotherms show metamagnetic behavior that is characteristic of non-collinear magnetic systems. Magnetization does not saturate even at lowest temperature in 9 T field with negligible coercivity. The μ_{9T}/Ni is only 54% of its free ion value even at 2 K, which further supports presence of a complex non-collinear magnetic spin arrangement in this sample. The magnetic properties of this triclinic compound are drastically different when compared to its columbite type orthorhombic *Pbcn* structured counterpart.

m0026

Electrical Transport Properties of MoS_2/hBN Heterostructure Devices

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We describe the fabrication and electrical transport properties of field effect transistor (FET) devices made up of van der Waals heterostructure of layered two dimensional materials, MoS_2 and hBN on heavily doped $SiO_2/Si^{++,}$ where the Si acts as a global back gate and SiO_2 and hBN act as the gate dielectric. We characterize the channel material MoS_2 primarily with the PL spectra, which show strong excitonic features, suggesting it to be a monolayer. The transfer characteristics of the FET device, suggests that the channel is bipolar. The output characteristics at low temperature shows typical behavior for a semiconductor with a metallic contact. The linearity near the zero excitation was used to find the conductivity of the channel which varies in an activated manner with temperature for all the gate voltages. The low temperature activation energy was found to be varying from 15 to 20 meV over the gate voltage range. At higher temperature (>200 K) the system behaves as a bad metal.

m0027

The Waste Water Management Through Photodegradation of Methylene Blue: By Graphene-based Metal-oxide Composites

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Abstract. With the motto "every drop matters: and wastewater can be an alternative resource", Cost-effective, accessible technology has been developed to refine wastewater by degrading harmful chemicals like methylene blue and organic dyes. In this regard, the main focus of this research is how graphene-based nanocomposites affect the degradation of dyes using sunlight. Here, zinc oxide nanoparticle (ZnO NP) inside GO composites plays an essential role in the photodegradation of MB. The catalytic activity of GO (32% in 1hr) is enhanced to (82% in 1hr) for GO@ZnO composites. Photodegradation of MB is even more dramatic when the iron nanoparticle is incorporated inside GO composites resulting 99% of degradation (5% Fe-doped GO@ZnO) at 1 hr. The electron-hole recombination rate inside the GO composites can be regulated by incorporating ZnO and Fe, influencing the photodegradation process. The degradation of MB is nearly 96% by the Fe-doped composites upon testing in the actual sample using river water. Thus, synthesized composite is a potential candidate for being an effective adaptable photocatalyst for removing organic dyes from wastewater because of its excellent stability and reusability.

m0028

Optimization of MoS_2 nanosheets and MoS_2-Ag composites with Ag Nanoparticles for SERS Applications

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Abstract. Transition metal dichalcogenides (TMDCs) have seen tremendous growth in their synthesis methods and applications as well as in recent years. MoS_2 is one such material which has found application in various fields such as biosensors, superconductors, transistors, and many mechanical applications. Further, MoS_2 has also been explored as a potential candidate for surface enhanced Raman spectroscopy application. We have optimized the synthesis process for MoS_2 nanosheets morphology by the facile hydrothermal method. Different reaction parameters were tuned to synthesize the single and separate MoS_2 nanosheets with distinct boundaries. Prepared nanosheets were characterized using the FESEM, Raman, XRD, UV-vis spectroscopy. RhB is a carcinogenic dye which has life-threatening effects and therefore prohibited to use in food items. RhB is still used as a food colorant and its detection is important. The final product of MoS_2 nanosheets was used as a surface enhanced Raman spectroscopy (SERS) substrate to detect the RhB dye up to a concentration of 10^{-8} M. These nanosheets were further functionalized with Ag nanoparticles to increase the sensitivity and limit of detection of the MoS_2-Ag

nanocomposite SERS substrate. Nanocomposite SERS substrate successfully detects the ultralow concentration of 10^{-14} M of RhB dye. Thus, nanocomposite of MoS_2 and Ag NPs can be used as an effective SERS substrate for RhB and other harmful dyes.

m0029

Hydrogen Adsorption on Au-BL-MoS2 Hybrid Surface: an Ab-Initio Study

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Hydrogen adsorption is a fundamental and elementary reaction that plays a crucial role in Hydrogen production for the global transition to a more sustainable energy future. In this regard, the TMDCs have been studied extensively as an electrocatalytic material due to their tunable property and large surface area for H adsorption. In this work, we explore the possibility of a Bilayer (BL)-MoS_2-Au hybrid for enhancing the electrocatalytic activity through Hydrogen Evolution Reaction using first principle calculations. We have obtained an optimum H adsorption of -0.34 eV for the BL-MoS_2-Au hybrid which is within the accepted range for HER. We have performed the Bader Charge Analysis and Charge density difference calculations which further validate the improved catalytic activity of BL-MoS_2-Au hybrid for HER applications.

m0030

Two Dimensional Mn/Zr-BDC Metal Organic Framework for Dye Adsorption

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Here in we report the room temperature solvothermal synthesis of two dimensional bimetallic (Mn & Zr) benzene di-carboxylic acid based metal organic framework. The two-dimensional bimetallic metal organic framework material was characterized by PXRD, SEM and FT-IR. The prepared compound is also studied for the room temperature organic dye removal from water medium at neutral pH.

m0031

Intrinsic Material Properties of Two-dimensional Rb_2Se Monolayer via DFT Simulations

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Abstract. In this study, the theoretical predictions of rubidium sulphide monolayer are performed via the first principles approach. Herein, the trigonally crystallizing Rb_2Se monolayer(s) electronic band structure and effective mass curve is primarily discussed. By the means of DFT computations it is found that the material is a semiconductor with 1.56 eV electronic bandgap and has dominant positive charge carriers m_{eff}^{h}.

m0032

Theoretical Investigation of 2D Rb_2O Monolayer: A DFT Study

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Abstract. 2D materials possess enchanting properties that are distinct from their counter bulk part due to the quantum confinement effect. Both experimentally and theoretically, Researchers all over the world have been investigating 2D materials. In this research, the 1T phase of the Rb_2O monolayer was investigated by employing Density Functional Theory (DFT). The structural and electronic properties were studied utilizing the WIEN2k software. The relative ratio (D) of the Rb_2O monolayer is also calculated to calculate the transfer efficiency of the electron-hole pair.

m0033

Optoelectronic Properties of van der Waals Heterostructure WS_2/Bi_2Se_3

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Abstract. Recent research has extensively examined the structural, electrical, and optical characteristics of the WS_2/Bi_2Se_3 van der Waals(vdW) heterostructure using the density functional theory method. This heterostructure material's electronic characteristics, including the anticipated electronic band-structure and state density, as well as those of its component materials WS_2 and Bi_2Se_3, have all been investigated. Using the Random Phase Approximation, the optical characteristics of the heterostructure WS_2/Bi_2Se_3 have been investigated Independent Particle Approximation (IPA). According to the results, WS_2/Bi_2Se_3 van der Waals (vdW) heterostructure is a promising material for nano- and opto-electronic devices.

m0035

Halogen Modification of $M–N_6$ Single-Atom Catalysts for Enhanced Electrocatalytic Hydrogen Evolution Reaction

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Abstract: The quest for sustainable energy solutions has emphasized the pivotal role of the Hydrogen Evolution Reaction (HER) in generating clean and efficient fuels. Single-atom catalysts (SACs) have emerged as promising contenders, renowned for their impressive catalytic activity, stability, and efficient utilization of transition metals. Notably, the utilization of single metal atom-based catalysts offers the potential to significantly reduce catalyst costs by maximizing activity with minimal metal usage. This potential hinges on stabilizing metal atoms as individual active sites within supporting materials. Theoretical considerations highlight graphitic carbon nitride (g-C3N4) as a viable candidate for hosting single transition metal atoms, positioned at the central voids between heptazine units. Intriguingly, these metal atoms within the voids coordinate with six neighboring N atoms from the surrounding heptazine motifs. Our study delves into the HER activity of stable metals—V, Cr, Mn, Zr, and Nb—introduced into the structure of graphitic carbon nitride (g-C3N4). We investigate the modulation of metal site activity through halogen, specifically Cl-, and uncover that Cl-modified metal sites can enhance HER activity for specific metals such as Nb and Zr, while eliciting a repulsive effect for others.

t) Thesis papers

t0003

Compaction of ct-DNA by Gemini Surfactants with Variable Spacers and SiO_2 Nanoparticles and its Applications towards *in vitro/in vivo* Gene Delivery

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Abstract. Compaction of calf thymus DNA (ct-DNA) by two cationic gemini surfactants, 12-4-12,2Br^- and 12-8-12, 2Br^- in the absence and presence of negatively charged SiO_2 nanoparticles (NPs) has been explored using various techniques. 12-8-12,2Br^- having a longer hydrophobic spacer induces a greater extent of ct-DNA compaction than 12-4-12, 2Br^-, which becomes more efficient with SiO_2 NPs. Fluorescence lifetime data reveal the binding sites of surfactants to ct-DNA. Fluorescence microscopy and flow cytometry are performed for *in vitro* cellular uptake of YOYO-1-labelled ct-DNA with surfactants and SiO_2 NPs using 4T1 cells after 3 h and 6 h incubations. The *in vivo* tumor accumulation studies are carried out using a real-time *in vivo* imaging system after intravenous injection of the samples into 4T1 tumor-bearing mice. 12-8-12 with SiO_2 has delivered the highest amount of ct-DNA in cells and tumors in a time-dependent manner. So, the application of a gemini surfactant with SiO_2 NPs in compacting and delivering ct-DNA to the tumor is proven, warranting its further exploration for cancer treatment therapy.

t0004

Vibrational And Structural Investigations Of Phase Transitions In Vanadium Based Framework Oxides

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Abstract: A thorough investigation of the structure and dynamics of a large series of vanadium oxides of the $A_3(VO_4)_2$ family (A = Ni, Co, Mn, Mg or for the more complicated $BaCu_2$ and $Li_{0.2}Mn_{2.9}$ forms) and the related $Zn_4V_2O_9$ compound is investigated in combination of in-house high-pressure Raman spectroscopy together with high-pressure X-ray diffraction (XRD) done at synchrotron. The Raman spectroscopic investigation of $Ni_3(VO_4)_2$, $Co_3(VO_4)_2$, $Mg_3(VO_4)_2$, lt-$Mn_3(VO_4)_2$, $Li_{0.2}Mn_{2.9}(VO_4)_2$, $BaCu_2(VO_4)_2$ and $Zn_4V_2O_9$ at different thermodynamical conditions (pressure and temperature) to identify anomalies in the observed Raman active modes which is later investigated with synchrotron XRD investigations. Overall, the highlighted findings of the present research work are the discovery of the new high pressure phases of lt-$Mn_3(VO_4)_2$, $Li_{0.2}Mn_{2.9}(VO_4)_2$ and $Zn_4V_2O_9$ which are majorly characterized with Raman spectroscopy. Here, I present overview of the detailed experimental findings and the complimentary nature of the two techniques on the observed anomalies in structure and dynamics for the same class of compounds.

t0005

Optoelectronic Applications and Spintronic Aspects of Metal Halide Perovskites

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The overreaching objective of this doctoral thesis was to study the optoelectronic and spintronic properties of several metal halide perovskites towards their device applications. Despite the success of $MAPbI_3$ in optoelectronics, specifically in photovoltaics, two major concerns could be found. The stability issue of the compound and the toxicity of lead have triggered the research thrust to find alternate materials in the field of perovskite optoelectronics. In this context, the motivation of the research work in the first part of the thesis was to address one focal question: "Is there any alternate perovskite beyond $MAPbI_3$ for viable photovoltaic applications with better stability and probably less toxicity?"

In the next part of the thesis, spintronic aspects of these materials were investigated. Finally, the goal was to address one pivotal question: "Can we integrate optoelectronic and spintronic properties of metal halide perovskites for next-generation opto-spintronic devices?".

t0006

Fabrication and Characterization of Nano-structured Thin Films and Multilayers by Oblique Angle Deposition (OAD) Technique

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The oblique angle deposition (OAD) refers to a thin film deposition geometry where the vapour flux arrives at an oblique angle on the substrate surface. The present work describes systematic investigations on the tailoring of optical, morphological

and other related properties of nanoporous metallic (silver), dielectric (titanium oxide) and metal- dielectric composite (silver/titanium oxide) thin films fabricated using electron beam evaporation technique in OAD configuration for various applications such as anti-reflection coatings (ARCs), nanoplasmonic coatings etc. A novel collimated glancing angle deposition (collimated GLAD) technique has also been employed for extended tuning of the optical and morphological properties of the thin films. The TiO_x thin films prepared in collimated GLAD configuration has shown very low refractive index of ~1.101 (at 550 nm) together with single layer anti-reflection (SLAR) coating characteristics. A multilayered anti-reflection coating (ARC) fabricated from a single material of TiO_x has shown ~98.5% optical transmittance in the visible wavelength region. A critical substrate temperature to achieve sharp plasmonic absorption in Ag thin films has been demonstrated. Film thickness and post deposition annealing induced sharpening of LSPR absorption has also been achieved. A spatially selective nanoplasmonic resonance has been demonstrated for Ag/TiO_x nanocomposites across the substrate.

t0007

Sodium *p*-Nitrophenolate Dihydrate and Sodium 4-Nitrophenoxide 4-Nitrophenol Dihydrate Single Crystals for NLO and Terahertz Applications

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The basic concepts of the crystal growth and experimental procedures, instrumentation part is described in the first chapter. The potassium 4-nitrophenoxide 4-nitrophenol dihydrate single crystal growth and their structural spectroscopy, optical, thermal, and NLO properties are studied in Chapter II. The sodium *p*-Nitrophenolate dihydrate single crystal growth and their structural, spectroscopy, and nonlinear optical properties are studied. The THz-TDs behavior is studied using Ti-sapphire laser source of 808 nm interaction is explained in Chapter III. The sodium 4-nitrophenoxide 4-nitrophenol dihydrate single crystals structural, spectroscopy, nonlinear behavior. THz-TDs measurement, the refractive index is studied using femtosecond interaction in Chapter IV. The inclusion free (010) orientation of $NPNa.2H_2O$ single crystal of 6.5 cm is grown from SR method. Phase purity of the composition is studied with powder xray diffraction studies. The third-order NLO behavior of $NPNa.2H_2O$ single crystal is studied to identify the refractive index given in Chapter V. Piperazinium – 3,5 dinitrobenzoate single crystal growth, Characterization and their third order NLO properties are studied. further way of approach is given in Chapter VII.

t0008

Growth and Characterization of Doped Organic and Semi-organic Single Crystals for Linear and Non-Linear Optical Applications

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Abstract. High quality bulk single crystals with enhanced properties for scientific, technological and industrial applications can be grown by adopting several methods. 2, 4-Dinitro phenol (DNP) and Malachite green (MG) dye doped tris thiourea zinc –II sulphate (ZTS) single crystals as well as L- Phenylalanine (L-Phe) doped potassium dihydrogen Phosphate (KDP) were effectively grown by employing a straightforward, simple and cost effective slow evaporation solution technique (SEST). Diffraction curves recorded for 0.1 mol% 0.2 mol% and 0.3 mol% of 2,4 DNP doped ZTS specimen crystals showed relatively low full width at half maxima (FWHM) values which reveal the successful growth of doped ZTS for enhanced photonics applications. The results of second harmonic generation (SHG) studies revealed that the SHG efficiency was increased by 2.75 times with MG doping in ZTS crystals. The intensity of emission peaks at ~313 *nm* and ~616 *nm* decreased with increase in doping concentration of L-Phe in KDP crystals. The PL intensity is highest for the doped specimens (at ~313, ~366 and ~470 *nm*), indicating the existence of F-centres or colour centres due to oxygen vacancies as observed. The maximum intensity at lower doping concentrations of L-Phe doped KDP crystals indicates highest improvement in quality of this sample among the others. Single crystals of novel organic compound of 4-chloro 3-nitrobenzophenone (4C3N) was grown in the laboratory by SEST and Sankarnarayanan – Ramasamy (SR) methods from acetone as solvent medium. The photolumniscent spectra revealed red shift in the emission peaks of grown crystals which are in good coherence with UV- Visible spectra. HRXRD characterization was utilized to see the nature of perfection of grown 4C3N crystals. On comparison of FWHM values of SR and SEST-grown crystals revealed the superiority of SR-grown crystals, which could be responsible for the enhancement of optical transparency of SR grown crystals.

t0009

Photoemission Study of Quasiperiodic and Chalcogenide Substrates and Adlayers

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In this thesis, we employ photoemission spectroscopy (PES) to investigate the electronic structure of aperiodic crystals lacking translational symmetry. We mainly focus on the bulk electronic structures of quasicrystals (QC) that exhibit long range order without any translational symmetry, and related quasicrystalline approximants that are periodic but show similar atomic arrangements resembling QCs, studied using hard X-ray PES (HAXPES). Additionally, charge density wave (CDW) modulated layered rare earth tritelluride (RTe_3) single crystals e.g., $LaTe_3$ and YTe_3 are examined, with unidirectional incommensurate wavevector $\mathbf{q}_{CDW}$ that breaks translational symmetry. HAXPES analysis of quasicrystals such as icosahedral

(*i*) Al-Pd-Re and decagonal (*d*) Al-Ni-Co reveals pseudogap features at the Fermi level (E_F), that are theoretically predicted to stabilize these aperiodic structures via Hume-Rothery mechanism. Deeper pseudogaps in high-order approximants (Al-Pd-Cr-Fe and Al-Pd-Mo-Fe) have been found in comparison to their related *i*-Al-Pd-Mn QC. Surface-sensitive PES techniques and low energy electron diffraction (LEED) have been utilized to investigate quasiperiodic adlayers (Sn and Te) grown on QC substrates, showing pseudogaps at E_F. A combined study using ARPES and density functional theory on non-magnetic $LaTe_3$ and YTe_3 reveals CDW-induced Kramers nodal lines in their electronic band structures. ARPES, LEED, and scanning tunneling microscopy confirms the presence of twin domains with perpendicular CDWs in YTe_3.

t0010

Probing Nanoparticle-Surfactant Complexes Using Scattering Techniques

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Abstract. The synergistic effects of nanoparticle-surfactant complexes depend on the resultant structure as well as on the interplay of nanoparticle-surfactant, nanoparticle-nanoparticle, and surfactant-surfactant interactions. This work provides an understanding of these interactions along with the resultant structures which are formed as a result of this nanoparticle-surfactant conjugation. Studies have been carried out employing a system of charged nanoparticles and both charged and uncharged surfactants, where their conjugation is governed by the selection of surfactant, modifying solution parameters (alcohol as an additive and ionic strength), and altering nanoparticle size.

t0011

Multi-scale modeling of high strain rate deformation and spall fracture in poly-crystalline metals

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Dynamic-response of materials at high strain rates is being investigated using Molecular Dynamics (MD) to understand the underlying physical phenomena in a material under impact-shock-loading conditions. MD is used to obtain shock and fracture parameters data at the atomic length (10-100 nm) and time (1-100 ns) scales for the materials under high strain rates. This research work is focused on the single-crystal and bi-crystals of metals and their response to high velocity impact. The highlight of this work is the application of the multi-scale method to obtain fracture parameters in single and polycrystalline metals. The multi-scale method involves sequential execution of (a) molecular dynamics, (b) multi-parameter optimization to obtain material-dependent fracture parameters and (c) one-dimensional hydrodynamic simulations to calculate the spall-fracture parameters. The problems investigated are: (i) impact-shock propagation in single and bi-crystals, and (ii) multi-scale method for single and bi-crystals, to calculate the spall fracture parameters. The results using the multi-scale method match experimental results of dynamic spall strength with an accuracy up to 95%.

t0012

Development of Highly Efficient Photocatalysts Based on Semiconductor, Ferroelectric and Plasmonic Heterostructures

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In this research work, we have tried to enhance the photocatalytic activity of semiconductor MoO_3 photocatalyst by integrating it with ferroelectric and plasmonic materials in order to benefit their individual properties. First, we tuned the photocatalytic activity of semiconductor MoO_3 via substrate temperature and obtained an efficiency of 31% for the degradation of rhodamine B dye (RhB) under 1 hour of UV-visible light illumination. In order to further enhance the efficiency, we have coupled ferroelectric $BaTiO_3$ (BTO) with semiconductor MoO_3. The BTO/MoO_3 heterostructure has showcased an improved efficiency of 86% in 1 hour of UV-visible light illumination for the degradation of RhB and is attributed to the combined effect of interface charge coupling and heterostructure band alignment. The surface plasmon resonance (SPR) of green synthesised silver nanoparticles (Ag NPs) is optimised and exhibited good bio-sensing as well as photocatalytic activity. The photocatalytic efficiency is further enhanced by incorporating green synthesised Ag NPs over the BTO/MoO_3 heterostructure. The BTO/MoO_3/Ag (BMA) ternary heterostructure exhibited a 100 % efficiency for the degradation RhB dye in 1 hour of UV-visible light illumination and is attributed to the enhanced interfacial electric field due to the formation of the electric double layer. A strong correlation has been established between structural, morphological, optical, electrical and photocatalytic properties of individual layers and heterostructures.

t0013

Theoretical Study of Electronic and Optical Properties of Quantum Dots

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Abstract. Graphene Quantum Dots (GQDs) have been investigated by tuning the bandgap and engineering the controlling parameters in order to analyse their use in optoelectronic applications. In order to tune the band gap and engineer their optical properties, such as absorption and emission spectra, passivation of dangling bonds of GQDs has been carried out with the help of electron-withdrawing substituent. Calculations have been performed by simulating these GQDs with Density Functional Theory (DFT) formalism with functional B3LYP/631G* using Gaussian 09 software. In addition to passivation, surface and edge-modified configurations of GQDs with boronic acid (-BCO_2) and borinic acid (-BC_2O) respectively, heteroatom-doped

hexagonal GQDs have also been studied. All these modifications effectively decreased the band gap of GQDs resulting in a redshift in the absorption spectra. Compared to surface-modified GQDs, the presence of a B atom in the edge-modified GQDs was found to have a pronounced effect on tuning the energy bandgap. Also, -BCO_2 affects the electrical structures of GQDs more significantly than borinic acid -BC_2O. The HOMO and LUMO topographical surfaces have been used to understand the absorption spectra. These surfaces showed some σ-bond characteristics along with π-bond properties in these GQDs, which further resulted in the alteration of their energies and a corresponding decrease in their band gap. In emission properties, the fluorescence of surface-modified GQD was found to fall in the near-infrared region with a quantum yield of 29 % rendering them suitable for bio-imaging applications. In the case of heteroatom doped-GQDs, the fluorescence emission spectra of all these GQDs established that their fluorescence peaks lie in the near-infrared region (NIR). Compared to other doped GQDs, sulfur-doped GQDs exhibit a considerable quantum yield of 26% with an emission wavelength of 850 nm (NIR-I). These results are expected to find significant applications in biological and optoelectronic applications.

t0014

Study of Structural and Ferroelectric properties of Perovskite Materials

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The present thesis is dedicated to lead free ferroelectric and magnetically driven ferroelectric materials. $BaTiO_3$ (BTO) is a well-known lead free ferroelectric materials with three structural phase transitions cubic to tetragonal around 403 K, tetragonal to orthorhombic around 278 K and orthorhombic to rhombohedral around 198 K respectively from high temperature to low temperature. We have investigated the effect of Sr doping on the structural, dielectric and ferroelectric properties of BTO. Structural correlation shows that TiO_6 octahedral distortion has dominant role in the dielectric and ferroelectric properties of Sr doped BTO. Second part of the thesis is dedicated to the study of magnetoelectric and multiferroics property of $Co_4Nb_2O_9$ (CNO) through detail temperature synchrotron X-ray diffraction, Raman spectroscopy and magnetodielectric studies of polycrystalline and single crystal of CNO.CNO is the one of the interesting magnetoelectric materials with antiferromagnetic ordering around 27.2K. Structural study shows that there is small lattice distortion at T_N mediated by spin-phonon coupling, which enhance in the presence of the magnetic field, as observed in temperature dependent dielectric measurement.

t0015

Thermodynamic Properties and Diffusion in Ionic Conductors

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Abstract: The ionic conducting materials are useful in energy storage devices such as batteries and capacitors. Achieving reasonable ionic conductivity (~mS/cm) at room temperature is challenging and very much required for future solid-state batteries. This requires a thorogh understanding of the diffusion mechanism. In this thesis, we extensively explore the role of phonons on ionic diffusion and ion transport properties in various ion conductors. Using inelastic neutron scattering (INS) and quasielastic neutron scattering (QENS) measurements, we investigated the atomic dynamics in various solids. The QENS measurements are useful for identifying the magnitude and nature of diffusion, such as the presence of localised vs long-range diffusion. To interpret the experiment results and get a microscopic understanding of ion transport in solids, we performed ab-initio lattice dynamics and molecular dynamics simulations. Using experiments and simulations, we identify the specific phonon modes that help in cationic hopping and may initiate diffusion. Further, these phonons enable us to understand the thermodynamics and transport properties at the atomistic level. We employed some strategies to enhance the ion conductivity, such as via creating doping, vacancy, and amorphisation. These strategies tune the free-energy landscape and provide a low-energy barrier for ion diffusion.

t0016

Physical Vapor Deposition and Characterization of Diverse Sb_2Se_3 Crystalline Morphologies

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Abstract. Tremendous development in crystal growth technology led to the production of good quality samples for the design and fabrication of optoelectronic devices. As naturally available solids exhibit undesirable characteristics, the present research work deals with the artificial synthesis and characterization of defect free binary layered chalcogenide materials (LCMs) for photovoltaic (PV) applications. Antimony selenide (Sb_2Se_3) and tin diselenide ($SnSe_2$) have gained special attention in the PV industry due to their eco-friendly, sustainable, and non-hazardous nature as well as the salient features such as moderate melting temperature, *p*-type conductivity with direct transition, optimum band gap and high absorption coefficient. Therefore, cost-effective synthesis was implemented to engineer bulk Sb_2Se_3 and $SnSe_2$ crystals for the enhancement of optoelectronic parameters. Single crystal growth from melt allows the fabrication of large size samples under controlled environment. It gives rise to complexities in maintaining stable temperature for crystallization and achieving chemical homogeneity, if multiple elements are present in the system. The challenges associated with Bridgman-Stockbarger and Czochralski methods for preparing bulk crystals include irregular heat flow, mechanical movement of furnace or crucible, thermal stress, etc. Moreover, reactivity of the melted material with the ampoule leads to structural irregularities. Hence, horizontal normal freezing (HNF), the facile and inexpensive melt growth technique was employed to explore the suitability of cleaved samples. Most of the

vapor phase synthesis methods, especially, the chemical vapor deposition (CVD) deteriorates material quality, which adversely affects the physical properties due to the presence of contamination or foreign elements. But, the physical vapor deposition (PVD) process is favorable as it offers feasible instrumentation and yields stoichiometric specimens with supreme quality and fine-tuned characteristics. The PVD method could provide the evolution of various habits under high vacuum, if the processing protocols are critically controlled in a growth chamber. Even though research work has been published on Sb_2Se_3 and $SnSe_2$ samples prepared by other techniques, an economically viable approach by physical means for harvesting stoichiometric crystals, which enable versatile optical properties, has not been developed so far. A possible growth mechanism to explain the formation of crystals was proposed and discussed based on the Kossel-Stranski-Volmer (KSV) model. The phase identification, chemical homogeneity and microstructural evolution of the samples have been investigated by utilizing different sophisticated characterization tools like PXRD, EDAX, XPS, optical microscope, SEM, and TEM. Thermogravimetric analysis was performed for accessing the phase transition and thermal characteristics. Vickers microhardness tester was employed to probe the mechanical characteristics of the samples and Hall effect experimental setup was utilized to examine their transport properties. The optical measurements were carried out by UV-Vis-NIR and PL spectrometers. The results obtained were analyzed systematically to assess the suitability of harvested products for photovoltaic applications.

t0017

Oxide Composite for High Temperature Thermoelectric Power Generation

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Abstract. Scientists are exploring alternative renewable energy sources in the current scenario of rapid energy demand. Thermoelectricity is a promising clean energy source that can convert waste heat directly into electricity without any carbon footprint, making it an attractive option for industries and power plants. $SrTiO_3$(STO) is considered potential n-type oxide thermoelectrics. However, it suffers from poor electrical conductivity and high thermal conductivity. The electrons in these complex oxides suffer from Anderson localization, giving rise to poor electron mobility and consequently suppressed electrical conductivity. We have shown a novel designing strategy of composite formation, where the presence of secondary phases such as CNT, graphite help in the delocalization of those electrons by boosting the mobility. This results in a manifold increase in electrical conductivity in STO based oxide. Further, the incorporation of graphite causes more than 30 % decrease in the lattice thermal conductivity. Debye-Callaway model demonstrates that the phonon-phonon Umklapp scattering is mainly responsible for reduced thermal conductivity. As a result, ZT of 0.68 at 1000 K has been achieved in STO-based composite with graphite. Further, we have also fabricated a 4-leg TEG prototype, where we have obtained remarkable power output of 2.52 milliwatts.

t0018

Novel Electronic Structures and Behavior of Dirac Fermions in Nonsymmorphic Kondo Lattice Systems

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Abstract. This thesis investigates the electronic structure of nonsymmorphic Kondo lattice systems, specifically cerium-based pnictides ($CeTX_2$ where T = Cu, Ag; X = As, Sb), using depth- and angle-resolved photoemission spectroscopies. Experimental results reveal significant differences in surface and bulk electronic structures. We discover a new feature in the Ce 3d spectra instead of the typical Kondo feature in these Kondo lattice systems which suggests deviation from the Gunnarsson-Schönhammer model. The angle-resolved study revealed the nonsymmorphic symmetry protected Dirac cone along with a diamond-shaped nodal line protected by C_{2v} symmetry. The velocity of the Dirac fermions in this system is found to be much higher than that even in graphene; the velocity reduces slightly due to the interaction with local 4f states. The discovery of deviation from typical impurity models for correlated systems, high velocity of topological fermions and their evolution due to hybridization with local 4f states, reveal a new paradigm in the field of Kondo systems exhibiting topological behavior and calls for new theory to capture the underlying scenario.

t0019

Development of non-noble metal based anode catalyst for methanol oxidation in direct methanol fuel cell

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The growing energy demand due to continuous consumption of fossil fuels leads to the development of alternative energy conversion devices. Direct methanol fuel cell is the emerging area of research due to abundance of methanol, easy transportation and storage and high energy density [1]. However, methanol crossover, carbon monoxide poisoning and high cost of platinum hinder its commercialization. In the present thesis, non-noble electrocatalysts based on reduced graphene oxide (rGO), poly(3,4- ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) and transition metal oxide have been developed for methanol oxidation [2, 3]. The ternary nanocomposite modified ITO electrodes show lower onset potential and high anodic current density and long-term stability after 1000 CV cycles. The large surface area and high electrical conductivity of rGO nanosheet, film forming capability of PEDOT:PSS and presence of redox state in transition metal oxide contribute to the enhanced electrocatalytic activity of the electrodes. The oxyhydroxides formed in alkaline solution act as electroactive media during methanol oxidation. The methanol oxidation process has also been studied by varying the concentration of methanol and scan rate in the present thesis.

t0021

Structural, Magnetic, Thermal, and Electronic-Ionic Conduction Properties of Naturally Grown Layered Transition Metal Oxides

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Abstract. The present thesis work comprises the study of two-dimensional (2D) magnetic systems having a variety of 2D magnetic lattices. Due to the reduction in the magnetic lattice dimensionality, the combined effect of geometrical spin-frustrations and quantum effects lead to diverse magnetic ground states and spin-excitation phenomena, which are highly dependent on the underlying magnetic lattice geometry. The present thesis work evaluates the role of the underlying crystal lattice geometry and their lattice distortions (having different quantum effects and geometrical spin-frustrations) on the diverse magnetic properties. Further, the layered materials are chosen in such a way that the magnetic layers are separated by intermediate *A*=Li/Na/K alkali ions alone in a layer, which provides excellent ionic conductivity. Such layered materials are suitable for the applications in rechargeable batteries. The present thesis work also evaluates the microscopic mechanism of ionic conduction and establishes a correlation with the underlying crystal structure with regards to its potential battery application.

t0023

Synthesis and characterization of inorganic materials for potential applications in neutron dosimetry

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Abstract. Crystalline Al_5BO_9, $LiMgBO_3$ and glass of lithium magnesium borate (LMB) with different dopants were synthesized by chemical methods, structurally characterized using host a of techniques and their potential applications for Thermoluminescence (TL) based neutron dosimetry were studied. Based on the variation of calcination temperature, a strategy has been demonstrated towards the tunable dual application of Al_5BO_9: Mn, Li nanophosphor in terms of both as a red-light emitting phosphor and a promising TL based neutron dosimeter specifically for high intensity thermal neutron fields (~10^{11} n/cm^2) typically used in Boron Neutron Capture Therapy (BNCT). Similarly, Al_5BO_9:RE^{3+} (Tb/Ce/Eu) phosphors were also explored and the best result was found for $Al_5{}^{10/11}BO_9$:Tb^{3+}. For personnel neutron dosimetry, after exploring different systems, $LiMgBO_3$:Tb^{3+} phosphor was developed for the first time which demonstrated 2.2- and 4.5-times greater neutron induced TL sensitivity and n/γ dose discrimination capability, respectively as compared to standard LiF: Mg, Ti dosimeter. Based on detailed EPR and PL studies the underlying TL mechanism was delineated. Most importantly, it satisfies ISO-21909 criteria in terms of neutron dose linearity, TL fading etc. for practical applications.

t0024

Compositional Variation And Depth Distribution In D.C./R.F. Sputter Deposited Ni-Ti Alloy Thin Films

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Synthesis and structural characterization of Ni-Ti alloy thin films of various composition and thickness in nanometer regime deposited by five different sputter configurations using magnetron sputtering system were investigated. Effect of different sputter configurations which includes type of targets (NiTi, Ni, Ti), sputtering power (RF, DC), mode (sputtering, co-sputtering) on the elemental composition and depth distribution within the thickness of the films were investigated. Various characterization techniques (SIMS, XRR, EDAX, EDXRF, XRD, GIXRD, XPS, RBS etc.) were utilized for structural characterization of films. It was observed that oxygen contaminations were found to be present at the surfaces, interfaces of NiTi/Si and within the bulk of films. The content of oxygen in the bulk of the films depends upon working pressure. Ni-rich, Ti-rich and equiatomic NiTi thin films can be synthesized by these sputter configurations with uniform depth variation of alloying elements and minimal oxygen contaminations. Ti-rich Ni-Ti thin film annealed at 550°C showed the formation of crystal structure with B2 (austenite) phase at higher temperature and B19' (martensite) phase at room temperature confirming the Shape memory effect.

t0025

DEVELOPMENT OF TOXIC GAS SENSORS (NO_2, H_2S, NH_3, Cl_2, CO etc.) FOR E-NOSE APPLICATION

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Abstract. The primary research goal of the present study was to develop an electronic nose (e-Nose) for the toxic gas detection. For this ZnO based e-nose has been effectively designed and demonstrated to distinguish between the toxic gas mixtures. Additionally, developed a comprehensive data acquisition and analysis system for the e-nose application. Suitable machine learning models employed to classify, identify and predict the specific gases based on their unique sensor response patterns. The outcomes of this research study include a set of optimized toxic gas sensors capable of detecting multiple hazardous gases with high accuracy and reliability. Unbiased confirmation of the results provided by a carefully chosen a set of pattern recognition algorithms. The e-nose system developed in this study will provide a cost-effective solution for gas monitoring in

various industrial and indoor environments. The findings of this study will contribute to enhancing safety measures, reducing human exposure to toxic gases, and improving the overall environmental quality.

t0026

First Principles Investigations on the Physical Properties of Equiatomic Quaternary Heusler Alloys

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The physical properties of the novel EQHAs are calculated using first-principles calculations. First principles calculations are a powerful means of acquiring a bird's-eye view of the physical properties of Heusler alloys. We employed the Full Potential Linearized Augmented Plane Wave (FP-LAPW) methods, which are included in the WIEN2k package, to perform first-principles calculations. WIEN2k is the most accurate simulation tool for performing electronic structure calculations. We performed several essential calculations, including structural, mechanical, and thermal stability; spin polarized electronic structure, including band structure and density of states for both spin states; spin polarization and magnetic moments in the presence of uniform strain; total and atomic resolved magnetic moments; and Curie temperature using the mean-field approximation. Finally, we analyzed the influence of spin-orbit coupling (GGA+SOC) on the electronic structure of all computed EQHAs due to the presence of heavier atoms such as Zr, Ru, Y, Yb, and La. The present theoretical investigations will throw some light on the prediction of novel spintronic materials.

t0027

Studies on Nonlinear Optically Active Polymer Composites

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This study explores the nonlinear optical behaviour of three different materials: ADP-doped PVA/PVP polymer composites, KDP-doped PVA/PVP polymer composites, and silk, a natural fibre. The z-scan experiment was conducted by following Sheik-Bahae et al.'s technique, revealing two-photon absorption characteristics. At 1064 nm, the NLO properties were determined, with values of $\sim 10^{-7}$ W/cm for nonlinear absorption coefficient (β), $\sim 10^{-20}$ cm^4/GW for two-photon absorption cross-section (σ_2), and optical limiting properties. Functional data analysis (FDA) was utilised to gain insights into the behaviour and correlation of ADP polymer and Silk samples, identifying samples with favourable properties. Furthermore, the study introduced a novel performance measure for polymer composites, assessing the KDP-doped polymer matrix to determine an optimal dopant concentration for enhanced performance.

t0028

Polymer Nanocomposites As Lead-free Diagnostic X-ray Shielding Materials: Preparation, Characterization and Attenuation Studies

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Abstract. In this work, lead-free nanocomposites of silicone polymer containing single and multinanofillers are developed using a room temperature solution casting technique. Of all the single and multinanofiller systems, polymer containing Gd_2O_3 and Bi nanofillers (A13 nanocomposite) is found to exhibit an improved X-ray attenuation property. It is found to be effective against both dental (50 keV X-ray photon energy) and lung CT (single frame, 125 keV) scan conditions, with a mass attenuation coefficient of 5.26 and 2.22 cm^2/g, respectively, where the improved X-ray attenuation property is attributed to the good interfacial bonding between the nanofiller and polymer matrix, dual K-edge effect and the uniform distribution of nanofillers. The experimental data were in good agreement with the theoretical calculations. This study shows that A13 nanocomposite is a promising X-ray opaque material for the protection of patients and operators, in the form of thyroid collars, gloves, aprons, etc., during diagnostic X-ray techniques.

t0030

Evaluation of Dielectric Constant of Liquids and Validation with IOT based Electronic System

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Studies of the dielectric constant of liquids with traditional methods have a profound impact on physical, chemical, and electronic properties requiring physical presence for its determination. Present-day technologies greatly influenced towards determination of such properties developing smart systems interfacing the experimental setup. Conventionally measurement of physical parameters of the dielectric constant electronically requires an electric circuit at a specified frequency with the electronic circuit design involving an AC bridge, Conventional bridge, and microcontroller base method. The present article attempts to design an internet-enabled system to measure dielectric constant operated at various frequencies of interest with good accuracy. Materials selected belong to the family of amines and nitrile compounds that tends to allow the interstitial position to be occupied during the formation of mixtures with uniformity. A frequency generator circuit constructed using the dielectric liquid-based capacitor is interfaced with the microcontroller. The interface is with implementing the program with

the designed system, and the measured parameters are displayed on the display unit and extended to the Internet of Things (IoT). The designed system is validated for dielectric constant with traditional methods and proved an efficient smart system useful for technological applications**.**

t0031

Effect of Nano Sized Features on the Thermoelectric Performance of Low, Medium and High Temperature Range Thermoelectric Materials

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Worldwide, nearly 60% of the energy is wasted in the form of heat energy, and harvesting this waste heat is a key area of research. Thermoelectric power generators (TEGs) can convert waste heat directly into electricity. However, these TEGs have relatively low conversion efficiencies, which can be increased by improving the material's thermoelectric (TE) performance. Also, the waste heat is generated from the heat source over the temperature length scale, i.e., from low temperature (room temperature) to high temperature range (>823K), and accordingly, TE materials are also classified as low temperature range (room temperature to 573K), mid temperature range (573K-823K) and high temperature range (>823K) materials. In this thesis work, we have demonstrated the incorporation of nanoscale features in the material and especially the coherent nano interfaces in the matrix that can enhance the thermoelectric performance of low, medium, and high temperature range TE materials..

t0032

Surface engineered stealth nanoformulations for cancer theranostics

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This thesis deals with the development of new surface functionalized nanostructured materials for advanced cancer therapeutics and diagnostics. A series of soft nano-assemblies such as PEGylated vesicles, magnetic nanoparticles and organic-inorganic hybrid nanostructures were demonstrated for specific applications in the area of targeted therapy and diagnostics. The in-house developed cost effective PEGylated stealth liposomal doxorubicin has shown tremendous potential in both *in-vitro* as well as *in-vivo* studies equally in syngenic and xenograft model. The curcumin loaded PEGylated lipid nanoparticles have shown selective induction of apoptosis to lung cancer cell lines with minimal normal tissue toxicity. The efficacy of various organic coating agents such as malic acid, tartaric acid, glutamic acid, cysteine and PEG in stabilizing the magnetic nanoparticles (MNPs) and improve the loading of multiple drugs for chemotherapy application was investigated. The tartaric acid coated particles (TMNCs) was designed to act as a single platform theranostic platform for obtaining chelator free bimodal (MRI/SPECT-CT) Imaging with combinatorial chemo-thermal therapeutic efficiency in human breast carcinoma. It has shown a very high T2 (r2=171 $mM^{-1}s^{-1}$) contrasting ability than the FDA approved ferumoxides (120 $mM^{-1}s^{-1}$) and ferumoxtran (65 $mM^{-1}s^{-1}$) as MRI contrast agents. Three sets of Fe_3O_4 based nanoformulations were also developed with dual drug loading capacity (Curcumin & Doxorubicin, Doxorubicin & Methotrexate and Doxorubicin and Nitric oxide) with enhanced cancel cell killing efficacy with reduction in multidrug resistance. Novel methodology has been devised to impart shape selectivity during the formation Fe_3O_4 nanoparticles (Cubic shape). A highly stable micellar based nano-formulation of curcumin was also designed to load as high as 50 mg/mL of curcumin for nasal drop application (which is still stable even after 5 years of preparation). So far this nanoformulation has been transferred to three companies as technology transfer document. Thus, the present work highlights the application of organic-inorganic hybrid nanostructures for affordable treatment of cancer.

t0033

Study of strain mediated control over Magnetism in Ferromagnetic/Ferroelectric composites and thin films

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Abstract: Here, we have studied the strain-mediated magnetoelectric (ME) coupling in ferromagnetic (FM) and ferroelectric (FE) heterostructure in the form of both composites and thin film. The strain-mediated ME coupling in 3-0 type particulate composites such as; (1-*x*)PMN-PT:*x*CFO, and (1-*x*)PMN-PT:*x*CFREO (RE = La^{3+} and Eu^{3+}) with the concentration of ferrites *x* = 10, 15, 20 and 30 mol% has been investigated. When composites are placed under the influence of the magnetic field, they induce mechanical strain due to the magnetostriction behaviour of the ferrites, which are transferred to the neighbouring FE phase via the interface. The strain leads to the output voltage due to the converse piezoelectric effect of the FE phase (Magnetic Field ↔ Strain ↔ Electric Polarization). Each composite with an 80:20 ratio is found to exhibit the highest ME coupling coefficient (α_{ME}) in the range of 3.10 to 4.30 mV/cm-Oe (at 1 kHz, 300 K), and the value of α_{ME} further increases with increasing frequency, reaches up to a 3120 mV/cm-Oe of this off-resonance value at a resonance frequency. In addition, energy harvesting application is demonstrated for these composites by placing the sample atop the rotating AC axial exhaust fan. The 80PMN-PT:20CFLO composites show the highest V_{pp} of about ~4.24V at off-resonance mode. The results suggest that the studied composites could be effectively used as energy harvesters. Further, we have studied the strain-mediated control of magnetism by growing LSMO and PMN-PT thin layers on (001) oriented LAO single crystal substrates. Magnetization of the LSMO layer substantially enhances and dramatically decreases due to bi-axial strain induced on LSMO by the top PMN-PT layer and bottom LAO substrate.

t0034

Computational Studies of Shock Induced Effects In CHNO Compound

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Numerical studies have been performed to investigate (i) shock wave propagation along X, Y, and Z axes direction, (ii) the role of void in hot-spot formation during shock propagation, and, (iii) decomposition mechanisms, in RDX crystal. Shock wave propagation in RDX crystal is studied using reactive Molecular Dynamics (MD) simulations using the ReaxFF potential, and the effect of crystal anisotropy on shock wave propagation is investigated. The hot-spot formation is also explored through reactive MD. The decomposition mechanism is investigated using both, reactive MD wherein RDX is subjected to high velocity impact, and, using Kinetic Monte Carlo (KMC) when RDX is subjected to various pressures and temperatures. The novel aspects of this work are (i) the application of stochastic method such as KMC for studying the decomposition in RDX and comparison with the reactive MD, (ii) the study of crystal anisotropy on shock wave propagation, and (iii) comparison of the results obtained from numerical investigations of hot spot formation in RDX crystal and non-energetic material, copper to show that hot spots form at voids in both cases.

t0035

Synthesis and physical properties of alkaline earth metal doped $La_{9.67}Si_6O_{26.5}$ oxyapatite solid electrolyte

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One of the crucial hurdles to achieve high- performance SOFC systems is the electrolyte. Researchers are intrigued by the high oxide ionic conductivity of apatite-type lanthanum silicate oxide materials, which is equivalent to typical oxide ion conductors such as yttria stabilized zirconia. With the general formula $La_{9.33+x}Si_6O_{26+1.5x}$ $(x = 0-0.67)$, lanthanum silicate apatite (LSA) exhibits a high conductivity in the intermediate temperature range and a high oxygen transference number over a broad range of oxygen partial pressures. The apatite based FOICs (discovered by Nakayama in 1995) showed high ionic conductivity like perovskite based FOICs in low temperature regime (LTR). Among these FOICs, due to its anisotropic ion conduction $(\sigma_c^{\parallel}/\sigma_c^{\perp} > 10)$, lanthanum silicate oxyapatite is most interesting and attracted the researcher. in the present thesis, we are investigating the alteration in the structural and dynamics disorder with various substitution in the LSO. Alkaline earth and Rare earth substitutions at A-site have been done in order to improve the conductivities.

t0036

Magnetic Properties of Co-Cr-Al Based Heusler Compounds

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In the thesis work, the magnetic properties of $Co_{2-x}Cr_{1+x}Al$ (x = 0, 0.2, 0.4, 0.6, 0.8, 1) and $Co_{1+x}CrAl$ (x = 0, 0.25, 0.5, 0.75, 1) Heusler compounds have been investigated. All Co-Cr-Al based compounds have formed in Heusler compound-like *fcc* structure along with B2 disorder. A detailed study of magnetic properties reveals that all compounds show paramagnetic to ferromagnetic (PM-FM) transition. Below their PM-FM transition temperature, all compounds are soft ferromagnetic materials. The PM-FM transition temperature (T_C), saturation magnetization (M_S), the value of maximum magnetic entropy change ($-\Delta S_M^{max}$) under the application of a magnetic field (for $Co_{2-x}Cr_{1+x}Al$ series) and the value of relative cooling power (RCP) increase with increasing Co concentration within the compounds. Magnetic clusters within the paramagnetic matrix are observed for Cr_2CoAl, $Co_{1.2}Cr_{1.8}Al$, CoCrAl and $Co_{1.25}CrAl$ compounds. The values of critical exponents (β, γ and δ) associated with magnetic phase transition are unconventional for $Co_{2-x}Cr_{1+x}Al$ (x= 0.2, 0.4, 0.6) compounds. At very low temperatures because of the high strength of random anisotropy, the magnetization of the correlated region may freeze into the glassy state for Cr_2CoAl and CoCrAl compounds.

t0037

t0038

Synthesis and Study of Metal Oxynitrides Thin Films for Anticorrosive Applications

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Material corrosion is degradation of properties and functionalities, which in-turn invites various kinds of mutations in products, processes, quality and impact on nature. Different solutions to the problem were identified through interdisciplinary research, but the efficient, convenient and cost effective way is anticorrosive coatings. Among the group of organic and inorganic coatings, metal oxynitride coatings are novel and effective as integration of inherent properties of metal oxides and nitrides.

Here, investigations of transition metal oxynitrides (i.e. Tantalum, Vanadium and Titanium) were carried out with different corrosive environment and conditions. All these metal oxynitrides were acting as barrier to the corrosive species and preventing their access to the surface of substrate metal. Tantalum oxynitrides exhibits additional qualities like high hardness and

hydrophobicity. Vanadium oxynitrides are moderately effective among the group, where titanium oxynitride are efficient in prohibiting the percolation of chloride ions. Coatings with optimized properties are resulting into effective solutions to the corrosion problem.

t0039

Synthesis and Studies of Transport & Magnetic Properties of Nanostructured Materials

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This article reports exchange bias (EB) effect observed in different magnetic systems and the influence of some novel parameters on this particular phenomenon. A thorough investigation is performed on single-phase oxide sample $CoCr_2O_4$ in order to understand the influence of different parameters like, interparticle separation, variation of particle size, and surface effect on its overall magnetic properties. Investigation has been done and reported to understand the effect of interparticle interaction on EB phenomena for core-shell nanostructures in detail. A significant part of this article explores the magnetic and transport properties of graphene-based nanocomposites and thin film.

t0040

Magnetocaloric Effect Near Room Temperature with Wide Temperature Window and Critical Exponents Across the Magnetic Transition on Heusler Alloys and Composites

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In search of rare-earth free, low-cost, environment-friendly, hysteresis-free, broad working temperature near room temperature magnetic refrigerant, several Co and Ni-Mn-based Heusler alloys and composites have been explored in the thesis. The MCE value is quite large in the ordered Co_2TiSi as compared to the disorder Co_2TiAl. Among the all studied samples in this thesis, the maximum hysteresis free ΔS_M is found to be -1.98 J/kg-K at 30 kOe field change with a large RCP of 235 J/kg for $Ni_{50}Mn_{27}Ga_{23}$. The presence of inter-martensite transition along with the magnetic transition or magneto-structural phase transition widens the range of working temperature. The introduction of an external perturbation i.e., nano-structuring affects the magnetic ordering and magnetocaloric properties of $Ni_{1.8}Mn_{1.2}Sn$. However, the working temperature gets widened for nano-crystallite sample. Another effort has been made to widen the working temperature by making composites of the magnetically soft alloy (Ni-Mn-Sn-based) and hard ferrite (Barium Hexaferrite). It is interesting to note that, in between the two magnetic transitions, the ΔS_M shows quite a large value over a wide temperature range as compared to the left and right descending parts.

t0041

Electrocaloric effect, Ferroelectric and Optical Properties of $A_{1-x}A'_xTiO_3$ (A= Ba or (Na,Bi) and A' = (Sr,Sm) or Sr Perovskite Materials

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Lead-free perovskite ferroelectric materials are dominating in the electronics market because of their environment friendly and having various intriguing properties which enable these materials to be used in various technological applications. Among all lead-free materials, Barium titanate (BTO) and Sodium bismuth titanate (NBT) are the most investigated materials because of the comparable ferroelectric, dielectric and piezoelectric properties to the lead-based compounds. These materials have the capability to be utilized in electrocaloric cooling refrigeration as well as in optoelectronic devices. However, they have some shortcomings such as high transition temperature, sharp transition, high optical energy gap, etc. To overcome from these obstacles, various solid solutions based on BTO and NBT were synthesized by solid-state reaction method to investigate their electrical and optical properties. Various foreign elements (isovalent/heterovalent) having a mismatch in ionic radius were substituted to enhance the physical properties of BTO and NBT and also the main aim is to reduce the transition temperature towards room temperature.

t0042

Toxic Gas Detection Based on Inorganic, Organic Materials, Their Composites and Allied Techniques

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Abstract: Adverse effects on human health and environment due to emission of toxic gases has increased in recent years as a result of rapid industrialization and vehicular exhaust that necessitated the real time detection below their harmless levels. Metal oxide semiconductors are recognized as potential candidates for chemiresistive gas sensors owing to their high sensitivity, stability, simple structure, fabrication and measurement. However, there are few challenges that include selectivity, humidity effects and high temperature operation. Various strategies like exploration of nanostructures, addition of noble metals, formation of homo, hetero junctions, use of hybrid materials are found to be advantageous to improve the sensor characteristics. Hence the thesis work encompasses the gas sensing characteristics of thin films and nanostructures of metal oxide semiconductors ZnO, SnO2 and NiO and improved sensing characteristics of SnO2 thin films via metal addition and p-n junction formation with inorganic, organic semiconducting materials. Appropriate characterization techniques like X-ray photoelectron spectroscopy, Kelvin probe etc were employed to elucidate the sensing mechanisms.

t0043

Investigation of Facet Evolution on Si Surfaces Bombarded with Xe Ions

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This study investigates the formation of facets on Si surface under Xe ion irradiation using an ion energy of 0.5 keV. By examining the effects of ion incidence angle (60˚ - 85˚), fluence (4.5×10^{18} to 1.35×10^{19} ions/cm^2), and temperature (RT to 200 ºC), we explore the evolution of facets. The roughness of the surface exhibits a unique trend, reaching to its peak at an ion incidence angle of 80˚, which leads to the formation of faceted structures. Additionally, temperature studies highlight the important role of temperature in enhancing facet arrangement. To support experimental findings, numerical simulation using Anisotropic Kuramoto-Sivashinsky (AKS) equation is employed. These simulations provide valuable insights into the dynamics of facet evolution, allowing us to better understand how curvature-dependent sputtering yield, dispersion, and diffusion collectively influence the formation and morphology of facets on the Si surface under Xe ion irradiation.

y) Young achiever award nominee's papers

y0001

Tuning the work-function and energy storage properties of vertical graphene nano sheets by surface functionalization

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Abstract: Vertical graphene nanosheets (VGN), the new form of graphene-based material drawing a lot of attention due to their potential applications in diversified fields. The VGN features 3D interconnected porous networked geometry with non-stacking morphology that bestows a large surface area with a high density of sharp edges and defects. Herein, plasma-assisted surface functionalization is adopted to engineer the surface chemistry, work-function (WF), and in turn, achieved super-wetting VGNs. Further, surface functionalization is found to manipulate the defect density and also controls the defect type (sp3 or vacancy). Additionally, the surface functionalized VGNs exhibit 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. The Kelvin probe force microscopy (KPFM) investigations confirm the WF tuneability of the VGNs toward both lower and higher values by surface functionalization, thereby opening up their potential usage as electron and hole transport layers, respectively in organic solar cell devices. A solid-state supercapacitor device of supper-wetting VGNs is fabricated and demonstrated their performance by lighting an LED.

y0002

Capitalized Adsorption and Dehydrogenation of Ammonia on Ru_{55}, Cu_{55} and $Ru@Cu_{54}$ Nanoclusters: Role of Single Atom Alloy Catalyst

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Hydrogen production by the catalytic decomposition of ammonia (NH_3) is an important process for several important applications which includes energy production and environmental related issues. The role of a single Ru atom substitution on Cu_{55} nano cluster (NC) has been illustrated using NH_3 decomposition reaction as a model system. The structural stability of $Ru@Cu_{54}$ NC has been evaluated with Ru_{55} and Cu_{55} NCs for comparison. $Ru@Cu_{54}$ prefers icosahedron structure (Ih) like Ru_{55} and Cu_{55} NCs with almost comparable average binding energies of -5.55 eV/atom. The adsorption of NH_x (x=0-3) on different adsorption sites of icosahedron $Ru@Cu_{54}$ NC has also been studied and the corresponding adsorption energies estimated. The site-preference investigation suggests that, NH_3 prefers to adsorb vertically to the $Ru@Cu_{54}$. Stable geometries of N and H atoms on the high symmetry adsorption sites of $Ru@Cu_{54}$ NC have been studied. Though N atom favors top and hollow sites, H atom prefers to stay in Ru-Cu bridge site along with the hollow sites. The adsorption energy of N on $Ru@Cu_{54}$ NC is found to be -5.38 eV, which is very close to the optimal value (-5.81 eV) of ammonia decomposition volcano curve. The reaction energies for stepwise H atom elimination from adsorbed NH_3 molecule has been estimated. The energetics calculations for the dehydrogenation of NH_3 suggest that $Ru@Cu_{54}$ NC can be a suitable catalyst.

y0004

Screening, Design and Understanding of Material Properties through Atomistic Simulations

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The quest for advanced materials with desired properties requires thorough screening of chemical space as well as understanding their complex relations between composition, process/mechanism, structure, and properties. Present study combines high throughput atomistic simulation based material screening and experimental validations to discover new materials with desired properties. Such screening strategies are implemented to screen thermal expansion/conductivity and melting temperatures in mixed oxides, single-phase forming high entropy alloys and mechanical, dielectric, piezoelectric, and ferroelectric properties in hybrid organic-inorganic perovskites. Further, structure-mechanism-property correlation is established by predicting unusual material responses under high temperatures and stresses, e.g., phase transformations pathways, negative/zero linear compressibility, negative piezoelectric response, immunity towards depolarizing fields, and Rashba-Dresselhaus spin splitting.

y0005

Investigations on Preparation and Properties of Various n-Type p-Types ZnO Thin Films and Fabrication of p-n Homojunctions

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Abstract. ZnO is one of the most promising transparent conductive oxide (TCO) materials due to its optical and electrical properties. For the development of ZnO based devices, such as light emitting diodes, laser diodes and photo detectors, it is necessary to have *n*-type and *p*-type TCO ZnO semiconductor thin films. In this thesis, the pure and doped ZnO thin films

have been deposited on glass substrate through solution route assisted spray pyrolysis technique. Choosing the appropriate dopants and doping method are very important for the fabrication of *n*-type and *p*-type ZnO with good optical and electrical properties. Based on these factors, two donors (Mo and Eu), two dual acceptors (Na-N and Ag-N) have been chosen as dopants. For obtaining high-quality *n*-type ZnO films, the investigation is also carried out on the substrate temperature and thickness dependence of physical properties. The property studies, such as crystal structure and phase analysis by X-ray diffraction (XRD), surface morphology of the films by scanning electron microscopy (SEM), surface roughness analysis by atomic force microscopy (AFM), optical transparency in the visible region by UV-visible spectroscopy, influence of defects by photoluminescence (PL) studies and nature of conductivity by Hall measurements has been performed. The EDX and elemental mapping analysis shows the presence and distribution of elements in the deposited films.

y0007

Engineering Interfaces for Manipulating Electronic Properties in Functional Materials for Sensors and Energy

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Naturally occurring materials are limited in their electronic performance and offer limited tunability due to various physico-chemical constraints. Therefore, novel functional applications require tailor made materials that are unlikely to exist naturally. Hence such materials may be realized with optimal designing of interfaces in function materials which helps in achieving improved performance in various (or given) applications. We have engineered interfaces across a wide range of class of solids including metals, semiconductors, alloys as well as their nanoscale and low dimensional counterparts for applications such as thermoelectrics power conversion, selective gas sensors, selective solar absorbers etc. Some of the examples includes, Graphene-AZO or ITO based transparent conducting oxide nanohybrids for thermoelectrics[1], Graphene-titania nanotubes[2] and TMDCs with high entropy alloys[3, 4] as 2D-1D or 2D-0D nanocomposites for room temperature and selective gas sensing devices, ultrathin W metal layer sandwiched between thin $CuCo_2O_4$ layers for microcavity enhanced solar thermal energy harvesting etc[5].

y0010

Influence of dilute Nb^{5+} & Fe/Co metal ions substitution in $Bi_{4.0}Sm_{1.0}Ti_4O_{15}$; n=4 layered Aurivillius multiferroics

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ABSTRACT: We report a comprehensive investigation of the multiferroic property of Aurivillius ceramics of BSTFCO ceramics. BSTFCO ceramics were prepared by using a solid-phase reaction method. The phase purity and crystallinity were confirmed by an X-ray diffraction study. Well-deformed plate-like grains with the predetermined thickness of microstructures of ceramics were determined by field emission scanning electron microscopy (FESEM). Saturated M-H loops and soft ferroelectric hysteresis loops (P-E loops) with fields dependent were studied. Co-substituted ceramics exhibited ferromagnetic behavior, attributed to mixed valences and double-exchange interactions. Promisingly, energy storage densities and energy loss were calculated, showing potential for ME-multiferroic sensors and energy storage applications.

y0011

Investigation of Thermal Transport Behaviour of 2D TMDs Using Optothermal Raman Spectroscopy

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Thermal transport of semiconducting transition metal dichalcogenides (TMDCs) play an immense role in next-generation electronic, photonic, and thermoelectric devices. Here, we demonstrate thermal transport behaviour of MoS_2 and $MoSe_2$ using optothermal Raman spectroscopy technique. We have synthesized different triangular MoS_2 film with varying layer numbers (1L to 5L) and two distinct morphologies (snow-like and hexagonal) of trilayer $MoSe_2$ over SiO_2/Si substrate via chemical vapor deposition (CVD) method. To provide insights into the nonlinear temperature-dependent phonon anharmonicity, a semi-quantitative model comprising volume and temperature effects is used, divulging the dominance of three-phonon and four-phonon scattering processes for thermal transport in prepared MoS_2 and $MoSe_2$ films. We further calculate the interfacial thermal conductance (g) and thermal conductivity (ks) of prepared MoS_2 and $MoSe_2$ using appropriate heat diffusion model.

y0012

In Exploration of Exotic and Novel Magnetic Materials

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Discovery and exploration are two parallel realms of condensed matter physics which fuel the technology manufacturing industries. The emerging and revolutionary technologies such as artificial intelligence and data sciences grounding on computer science cannot survive without fast transfer of data and large storage of data in a miniaturized memory chips. At this junction, the research that uncovers the magnetic and physical properties of magnetic materials to decide on their functionality and practicality for an aimed technology. Research contributions resulted from the investigations of varied magnetic materials/phenomena using indigenously available facilities over the last few years is presented.

y0013

The 2D VSSe Janus As Anode Material: Leveraging Charge Transfer And Electronic Properties

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Abstract. The development of high-performance anode materials has been a crucial focus in advancing energy storage systems. The Janus 2D materials, characterized by their distinctive structural arrangement and dual nature, have garnered significant attention due to their unique electronic and charge transfer properties. In recent years, Janus materials have emerged as promising candidates for anode materials in Li and Na ion storages. In which we studied VSSe 2D Janus monolayer systems, due to their low molecular weights, they help in the specific capacity of metal ions. In our case, we use Calcium and Magnesium as metal ions due to their abundance, low toxicity, and high charge density due to their divalent nature compared to Li and Na due to their monovalent nature. In this work, the study of charge transfer of Ca and Mg ions on VSSe monolayer via Bader charge analysis is performed to studied their electronic nature and orbital contributions of Ca and Mg atoms near fermi levels, and the adsorption of metal ions on the system is study via first-principles calculation. which indicate the VSSe is a better candidate for anode material as dual-ion storage in battery applications.

y0016

Studies on Magnetic Memory Effect and Exchange Bias of Nanostructured Materials

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This article reports studies of exchange bias (EB) and magnetic memory effect of nanostructured materials. Magnetic memory effects in spin-glasses (SG), superspin-glasses (SSG) and superparamagnetic (SPM) materials have been discussed in detail with protocols and mechanisms. The origin of time (t) and temperature (T) dependent magnetic memory effects in different classes of materials have been discussed starting from the nanoscale towards the bulk magnetism. Magnetic memory effects (T and t dependent) in field cooled (FC) and zero field cooled (ZFC) protocols are focused to understand the physics of ageing and rejuvenation in SG, SSG and SPM materials. Exchange bias mechanism in different metal-metal oxide core-shell structures and magnetically inhomogeneous materials are investigated. The dependence of EB with core-shell diameter ration and interparticle interaction are reported which provides a platform to tune EB for potential technological applications.

y0018

Title: Metal-Insulator Transition and Variation in Magnetic Properties of NiS via Strain Engineering

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The application of external strain is considered to be an effective tool to exhibit electronic and magnetic transition in transition metal compounds. Employing first-principle density functional theory + Hubbard U (DFT+U) approach, we investigated the possibility of such transitions in hexagonal NiS which exhibits a semi-metallic antiferromagnetic ground state at ambient condition. We found that the application of tensile strain gives rise to a metal-insulator transition, while compressive strain provides the ways to collapse local magnetic moment on Ni site. The dominant exchange couplings are calculated for various values of strain and the route for enhancing transition temperature is proposed. Our results is expected to enrich the understanding of magnetism in NiS.

y0019

Transport properties of thermally driven topological Josephson junctions

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Abstract. We explore how length and phase difference of finite size Josephson junctions control the charge and thermal current when biased by temperature gradient. To minimize the loss due to scatterings, our Josephson junction is placed at spin quantum Hall edges so that all processes other than Andreev reflection and normal transmission are prohibited. By tuning the phase difference, an asymmetry in the behavior of the transmission amplitudes with the phase appears and thus can induce a charge current in the junction. The amplitude of the charge and thermal current is sensitive to the size of two superconductors. The amplitude is higher for smaller sizes. For a given phase difference, the charge current can change its sign for a shorter junction. The heat current carried by the transmitted electrons is also controllable by the phase difference and the size of the junction. Thermal conductance will be lower for smaller superconductors and lower base temperatures. Our topological Josephson junction provides further insights into the study of thermal transport in the Josephson junctions.

y0020

Magnon-Phonon Coupling in Layered Antiferromagnet

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Abstract. We present a fully analytical model of hybridization between magnon, and phonons observed experimentally in magneto-Raman scattering in van der Waals (vdW) antiferromagnets (AFM). Here, the representative material, FePS3, has been shown to be a quasi-two-dimensional-Ising antiferromagnet, with additional features of spin-phonon coupling in the Raman spectra emerging below the Néel temperature (*T*N) of approximately 120 K. Using magneto-Raman spectroscopy as an optical probe of magnetic structure, we show that one of these Raman-active modes in the magnetically ordered state is a magnon with a frequency of 3.7 THz (~ 122 cm-1). In addition, one magnon band and three phonon bands are coupled *via* the magneto-elastic coupling evidenced by anti-crossing in the complete spectra. We consider a simple model involving only in-plane nearest neighbor exchange couplings (designed to give rise to a similar magnetic structure) and perpendicular anisotropy in presence of an out-of-plane magnetic field. Exact diagonalization of the Hamiltonian leads to energy bands which show that the interaction term gives rise to avoided crossings between the hybridized magnon and phonon branches. Realizing magnon-phonon coupling in two-dimensional (2D) AFMs is important for the verification of the theoretical predictions on exotic quantum transport phenomena like spin-caloritronics, topological magnonics, etc.

y0021
Insights into the Mott metal-insulator transition beyond the classic Hubbard model
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Abstract. The Mott-Hubbard transition is a paradigmatic phenomenon in the study of strongly correlated systems, where Coulomb interactions between electrons drive a metal-insulator phase transition. This transition has been extensively studied within the Hubbard model that successfully incorporates the competition between itinerancy and localisation. This work investigates the Mott-Hubbard metal-insulator transition in a three-orbital lattice model. We provide an analytical estimate of the critical interaction strength at which the transition occurs at zero temperature within a simplified version of the dynamical mean field theory. This estimate establishes a relation between the critical interaction strength and the lattice parameters. Finally, we recast the manybody self-energy calculated with dynamical mean-field theory in terms of the boundary Greens function of a non-interacting, semi-infinite auxiliary chain. In this work, as a preliminary study, we particularly investigate the metallic phase, although such a mapping is general and can be used to gain insight into the possible topological character of the Mott-Hubbard metal-insulator transition observed in this model. We discuss the possibility of understanding the Mott-Hubbard metal-insulator transition in the three orbital lattice model as a topological phase transition.

y0022
Optics and Magneto-optics of 2D materials: research and development
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Abstract. Progress in the solid-state physics and devices, specifically the field of low-dimensional semiconductors is driven due to a quest for understanding the laws of physics at nanoscale up to macroscopic levels. My career so far has involved investigating optical and magneto-optical response of low-dimensional materials. I had a strong focus on development of new magneto-optical spectroscopy techniques for high-precision and resource-efficient measurements. This manuscript summarizes some of my most favourite works where either I have acted as a principal investigator (PI) and/or the principal contributing author, for an application of Young Achiever Award of the Department of Atomic Energy. Most of the works discussed here have been of fundamental importance to the community working either in the area of semiconducting van der Waals materials of the type *MX*2 (*M* = Mo, W; *X* = S, Se, Te, Re), or in high-precision magneto-optical spectroscopy. A special focus is given on the works performed within India. A few examples discussed in this document are: 1) Development of a mirror-based magneto-optical Kerr effect (MOKE) spectroscope for highprecision measurements and high-precision measurement of effective exciton g-factors in 2D GaAs quantum wells, 2) Single-photon emitters in monolayer and multilayer WSe2, 3) Discovery of interlayer excitons in few-layer van der Waals semiconductors, 4) Discovery of excited-state trions in a van der Waals semiconductor monolayer, and 5) Development of a high-performance Faraday Rotation spectroscope for spatially-resolved high-precision spectroscopy on 2D semiconductors and magnets.

y0023
A Class of Exactly Solvable Hamiltonians for S=1/2 Quantum Magnets with Spinless Fermionic Excitations in Higher Dimensions
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Abstract. This contribution summarizes the main results of an ongoing work on exactly solvable Hamiltonians for quantum magnets. A class of Hamiltonians which supports fractionalized spinless fermionic excitations in dimensions greater than one is written down. A well-known one-dimensional example is that of S=1/2 spin chains with Luttinger liquid physics and spinless fermionic excitations that are also called spinons. A well-known two-dimensional example is that of Kitaev's S=1/2 honeycomb model with bond-dependent magnetic couplings which supports Majorana fermionic excitations. The class of models to be discussed here also exploits bond-dependent couplings in a different way to nonperturbatively stabilize spinless

fermionic spinons and also Majorana fermions. A detailed account of these results including all the supporting technical information is being prepared for publication elsewhere.

***TBA:** To be announced

Author Index

PROGRAMME – DAE SSPS 2023

	Day - 1 (Wednesday, 20 December)	Day - 2 (Thursday, 21 December)			Day - 3 (Friday, 22 December)		Day - 4 (Saturday, 23 December)		Day - 5 (Sunday, 24 December)
08:30-9:30	Registration	Session	A 1	A2	A 1	A2	A 1	A 2	A 1
9:30-11:10	*Inauguration*	9:30-11:00	Soft matter and Biophysics	Magnetism	Novel experimental techniques for condensed matter	YAA presentations	Surface and Interface Physics	*Thesis Presentations*	Spin liquids and low dimensional magnetism
			B. V. R. Tata	Anushree Roy	Sandip Ghosh	*Presentations for Young Achiever Award (YAA)*	Krishnakumar Menon		Narayan Mohanta
	Plenary-1: Deepak Dhar		Tapomoy Bhattacharjee	Saurabh Giri	Harish N S Krishnamoorthy		Indranil Sarkar		A. K. Bera
			Basavaraj M. Gurappa	*Contributed Oral Presentations k0019, k0021*	S.K. Sharma		Mayank Srivastava		*Contributed Oral Presentations k0024, l0025*
11:10–11:40	*High TEA*	11:00–11:30	*TEA*						
11:30-13:00	*Plenary-2:* D. D. Sarma	11:30–13:00	*Contributed Oral Presentations a0011, a0016, b0019, b0031, c0002, c0020*	*Contributed Oral Presentations c0021, c0027, c0119, d0042, e0006, f0005*	*Contributed Oral Presentations f0063, g0016, h0021, j0025, l0022, l0099*	*Presentations for Young Achiever Award (YAA)*	Single crystals and semiconductors	*Thesis Presentations*	*Poster Presentation*
	Plenary-3: Hari Srikanth						Bharat Jalan		
							R. Radhakrishnan Sumathi		
							Swastik Mondal		
13:00-13:15	*Group photo*	13:00-14:00	Lunch						
13:15-14:30	*Lunch*								
14:30-16:30	*Plenary-4:* Ashok K. Ganguli	Session	A1	A2	A 1	A 2	A 1	A 2	*Award Presentations and Concluding Session (14.00-15.00)*
		14:00-16:00	Strongly correlated system and Superconductivity	Novel materials for energy conversion & storage	Multifunctional materials	Topological materials	Physics at quantum scale and photonics	Advanced materials for energy and environment	
	Plenary-5: Srikanth Sastry		Pratap Raychaudhuri	Vivek Polshettiwar	Sugata Ray	Nitesh Kumar	Sushil Majumdar	Samaresh Das	
			Ajay K. Mishra	R. S. Dhaka	Tathamay Basu	Surajit Saha	Gopal Dixit	Mayank K Gupta	
	Plenary-6: S. M Sharma		*Contributed Oral Presentations g0022, m0012*	Arup K. Rath	D. Bhattacharyya	Srijani Mallick	Himanshu Singhal	Manju Unnikrishnan	
				Contributed Oral Presentations d0020, j0006	*Contributed Oral Presentations h0050, i0015*	*Contributed Oral Presentations e0039, l0057*	*Contributed Oral Presentations f0006, m0013*	N.S. Ramgir	
16:30-18:30	*Poster Presentation (including YAA)*	16:00-18:00	*Poster Presentation*		*Poster Presentation*		*Poster Presentation*		A: Yellapragada Subbarao Audi, A1 : Shivaji Auditorium
18:30-19:30	*Evening Talk-1*	18:00-19:30	*Cultural Programme*		*Evening Talk-2*		*Interaction with Sponsors*		A2: Mother Teresa Auditorium

Venue: GITAM Deemed to be University, Visakhapatnam, India