68th DAE Solid State Physics Symposium

December 18-22, 2024

Abstract Book

Organized by

Bhabha Atomic Research Centre
Mumbai, India

Sponsored by

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

Venue:

DAE Convention Centre, Anushaktinagar,
Bhabha Atomic Research Centre, Mumbai

डॉ. अजित कुमार मोहान्ती
Dr. Ajit Kumar Mohanty

भारत सरकार
Government of India

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

MESSAGE

It is a privilege to welcome the delegates of the 68th DAE Solid State Physics Symposium (DAE SSPS 2024) at Bhabha Atomic Research Centre (BARC) Mumbai during 18 – 22 December, 2024. This is one of the most important series of meeting in the field of condensed matter physics, which provides an excellent forum for discussing technological as well as theoretical advancements and cutting edge research being pursued in the field of condensed matter physics.

DAE Solid State Physics Symposium has a long legacy, present one being the 68th in the series and is a highly sought after national event in this scientific field. I believe that the 68th DAE SSPS will bring together renowned experts from India and abroad to deliberate on the exciting topics as reflected by the scientific program. The scientific program is well charted, which includes sessions on futuristic Quantum, superconducting and energy materials, while also discussing the latest scientific trends in traditional areas like phase transitions, dielectrics, soft matter, magnetism and surface science. I am personally delighted to see the interest of large number of students and young researchers delivering presentations in the form of posters, oral talks, young achiever presentation and best PhD thesis presentation category.

I hope that all the delegates of DAE SSPS 2024 will have fruitful discussions during the conference, which can be nurtured to scale greater heights in future scientific endeavors.

Ajit Kumar Mohanty

(Ajit Kumar Mohanty)

परमाणु ऊर्जा विभाग की सेवा में परमाणु
पऊवि DAE
ATOMS IN THE SERVICE OF THE NATION

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विवेक भसीन
Vivek Bhasin

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Director, Bhabha Atomic Research Centre
सदस्य, परमाणु ऊर्जा आयोग
Member, Atomic Energy Commission

MESSAGE

With great pleasure, I extend a warm welcome to all the delegates of the prestigious 68th DAE Solid State Physics Symposium (DAE-SSPS), being held during December 18 - 22, 2024, at Bhabha Atomic Research Centre, Mumbai. DAE-SSPS is the flagship national event in the field of condensed matter physics research and this year it has returned to Mumbai after being held at different parts of the country during the last few years.

Over the years, DAE-SSPS has become one of the most popular national events in the field of condensed matter physics, which provides an excellent platform to students, scientists and young faculty to discuss the frontline research topics in this field as well as showcase their own research and technologies. The whole scientific program has been categorized in twelve sub- topics, including phase transitions, soft matter, nano-materials, single crystals and glasses, thin film technologies, magnetism, superconductivity, energy materials and low dimensional materials etc. The organizers have received more than 750 manuscripts this year in various sub-fields, which is a testament to the huge interest of scientific community to register their presence. There will be nearly 50 lectures from eminent speakers from India and abroad. One of the key aspects of DAE-SSPS is dedicated sessions for various student presentations, in addition to a large number of presentations from researchers in Young Achiever and Best PhD Thesis category.

I am sure that this symposium will nurture several new ideas and long-term collaborations in various research fields of condensed matter physics.

09.12.2024

(Vivek Bhasin)

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भारत सरकार
GOVERNMENT OF INDIA
भाभा परमाणु अनुसंधान केंद्र
BHABHA ATOMIC RESEARCH CENTRE
भौतिकी वर्ग
PHYSICS GROUP

On behalf of the Physics Group of Bhabha Atomic Research Centre (BARC), it gives me immense pleasure to welcome the delegates of the "68th DAE - Solid State Physics Symposium (DAE SSPS 2024)" being held at the DAE Convention Centre at Anushaktinagar, Mumbai during December 18 - 22, 2024. The DAE SSPS holds a long legacy, and it is one of the most attended events in the field of condensed matter physics in India. Over the years, DAE SSPS is being held at various Universities/ Institutes across the country. This year, we are happy to bring it back to BARC, Mumbai.

Along with several current exciting topics of condensed matter physics like quantum materials, topological materials, soft matter, dynamics and extreme conditions physics, the technical program of the symposium covers all the traditional topics of solid state physics which continue to fascinate the scientific community, such as phase transitions, superconductivity, surface science, and theoretical physics. It is also my pleasure to announce that we plan to celebrate the 60 scintillating years of density functional theory, and a dedicated session has been scheduled for the same.

Continuing the trends of DAE SSPS, around 820 manuscripts were received this year, a number which boasts the strength and popularity of the symposium in the country. We are also eager to attend the evening talk by Prof. Santanu Chaudhury which would delve into the relationship between physics and Artificial Intelligence, the field which could bring a Nobel prize in 2024. Like always, students and young researchers are the backbone of the symposium, and I sincerely hope that all the participants get benefitted with the widespread scientific feast.

My colleagues from the Physics Group of BARC have worked hard under the leadership of Dr. L M Pant to put up a scientifically enriching program and arrange for all the hospitality. I look forward to meet all the delegates and attend the exciting presentations of the DAE SSPS 2024.

(S. M. Yusuf)

डॉ. एल. एम. पंत
Dr L.M. Pant

सत्यमेव जयते
भारत सरकार
Government of India

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

Message

Department of Atomic Energy - Solid State Physics Symposium (DAE SSPS), one of the most prestigious national meetings in the field of condensed matter physics is being held at Bhabha Atomic Research Centre, this year, the place of its conceptualization. It is a matter of pride that this year, we are hosting the 68th edition of DAE SSPS, which has maintained its glory and popularity for a long time, and has now become a tradition. The venue of the symposium is DAE Convention Centre and will be held during December 18-22, 2024.

This year, we have received nearly 850 manuscripts under various categories. Nearly 25 coordinators and around 350 reviewers from across the country helped to review these manuscripts. While all the traditional branches of condensed matter physics are being covered, we have also introduced the fields of current research interests, like quantum materials, dynamics etc. A total of 12 thematic categories were laid out, under which all the manuscripts were received. The response to PhD thesis and young achiever categories was also overwhelming. We have tried to provide a fine blend of plenary, invited and contributory oral & poster presentations. With great pleasure, I am happy to announce a special evening lecture on the intersection of Physics and Artificial Intelligence, which perfectly aligns with the endeavour to bridge traditional research with bright future.

I would like to acknowledge the efforts of the scientific secretaries, Dr. Jitendra Bahadur and Dr. Himal Bhatt, who have worked hard to chart out a scientifically enriching program, well spread over the 5 days. I must also acknowledge Dr. Ajay Singh, Local Convener, and his team, who have worked with great dedication towards local hospitality and smooth conduction of this program.

I wish 68th DAE SSPS 2024 a great success and sincerely hope that all the participants get benefitted from this symposium.

12th December 2024

Dr. L. M. Pant

Convener, DAE-SSPS-2024

BARC
भाभा परमाणु अनुसंधान केंद्र
BHABHA ATOMIC RESEARCH CENTRE

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V. A. Bambole	Mumbai Univ. Mumbai
V. K. Aswal	BARC Mumbai

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 and Semiconductor Physics

j) Magnetism and superconductivity

k) Energy materials

l) 1-D, 2-D and quantum materials

AWARD CATEGORIES

t) Best Thesis

YA) Young Achiever

Program Overview

Day 1: Wednesday, December 18, 2024

<table>
<tr><td>08:30-09:30</td><td colspan="2">Registration</td></tr>
<tr><td>09:30-10:30</td><td colspan="2">Inaugural Function
(Venue: Auditorium 1)</td></tr>
<tr><td>10:30-11:10</td><td colspan="2">PL-1: Satischandra B. Ogale, TCG CREST, Kolkata
Designing New Materials for the evolving energy landscape and sustainable development
Session Chair: Gianluca Ciatto, Soleil Synchrotron, France
(Venue: Auditorium 1)</td></tr>
<tr><td>11:10-12:00</td><td colspan="2">Group Photo and High Tea</td></tr>
<tr><td>12:00-12:40
12:40-13:20</td><td colspan="2">PL-2: Tanusri Saha-Dasgupta, SNBNCBS, Kolkata
Quantum Materials by Computation: Challenges & Opportunities
PL-3: Sanat K Kumar, Columbia University, USA
Fragmentation Concepts explain Nanoplastic Formation and Temporal Persistence
Session Chair: S. M. Yusuf, BARC, Mumbai
(Venue: Auditorium 1)</td></tr>
<tr><td>13:20-14:30</td><td colspan="2">Lunch</td></tr>
<tr><td>14:30-16:30</td><td>Session 1: Emerging Magnetic Materials
Session Chair: Narayani Choudhury, Lake Washington Institute of Technology, USA
(Venue: Auditorium 1)</td><td>Session 2: Soft matter and Biophysics
Session Chair: Sanat K Kumar, Columbia University, USA
(Venue: Auditorium 2)</td></tr>
<tr><td></td><td>IT-1: Pinaki Sengupta, NTU, Singapore
Spin-1/2 kagome Heisenberg antiferromagnet: New insights from Machine Learning approaches
IT-2: P. S. Anil Kumar, IISC, Bengaluru
Magnetic-field free switching of ferromagnetic layers through Interfacial engineering</td><td>IT-4: Sarika Bhattacharyya, NCL, Pune
Exploring the structural contribution to dynamics in supercooled Liquids
IT-5: Shankar Ghosh, TIFR, Mumbai
Crafting Perfection: Annealing a Granular Polycrystal
IT-6: S. Mitra, BARC, Mumbai</td></tr>
</table>

	IT-3:Indranil Das, SINP, Kolkata *Novel Magnetic & Electrical Transport in Non-coplanar Magnetic Textures* **Contributary presentations:** a0030, k0042	*Beyond Brownian Motion: Non-Markovian and Non-Gaussian Mechanisms of Molecular Diffusion in Complex Fluids* **Contributary presentations:** b0027, b0036
16:30-18:30	**Tea and Poster Presentation**	
	a0001 to a0006, b0001 to b010, c0001 to c0012, d0001to d0007, e0001 to e0004, f0001 to f0006, g0001 to g0006, h0001 to h0009, i0001 to i0011, j0001 to j0015, k0001 to k0013, l0001 to l0008, t0001 to t0033, y0001 to y0025	
18:30-19:30	**Evening Talk:** Santanu Chaudhury, IITD, New Delhi *Intersection – Physics & AI* **Session chair:** U D Malshe, BARC/RRCAT, Mumbai	
19:30	**Banquet Dinner**	

Day 2: Thursday, December 19, 2024

09:30-10:10	**PL 4:** Rajeev Ahuja, IIT Ropar *Computational materials science and its applications in the area of materials for energy* **Session chair:** K. Maiti, TIFR, Mumbai ***(Venue: Auditorium 1)***	
10:15-11:15	**Session 3: 60 Years of DFT** **Session Chair:** Rajeev Ahuja, IIT Ropar ***(Venue: Auditorium 1)***	**Session 4: Novel Physical Phenomena at Nanoscale** **Session Chair:** V. K. Aswal, BARC, Mumbai ***(Venue: Auditorium 2)***
	IT-7: Kapildeb Dolui, Cambridge University, UK *Accelerating the Discovery of Ambient-Pressure High-Temperature Superconductors through Ab-initio Structure Search and Machine Learning* **IT-8:** G. S. Vaitheeswaran, University of Hyderabad	**IT-11:** S. Dhara, IGCAR, Kalpakkam *Phonons at nanoscale* **IT-12:** Summet Walia, RMIT University Australia *Two-dimensional materials for next-generation electronics and optoelectronics technologies*

	Uncovering Multifold Phonon Degeneracies in Cubic Nb_3Bi	
11:15-11:45	**Tea Break**	
11:45-13:00	**Session Chair:** Nandini Garg, BARC, Mumbai **IT-9:** Saurabh Ghosh, SRM Chennai *Polarization Coupled Magnetization Switching in ABO_3 Oxides* **IT-10:** Kartick Tarafder, NIT Surathkal *The Non-Trivial Topological Landscape of 4D Transition Metal Systems* **Contributary presentation:** g0002	**Session Chair:** V. A. Bambole, Mumbai University **IT-13:** R. S. Ningthoujam, BARC, Mumbai *The Nobel Prize in Chemistry 2023: Discovery and Synthesis of Quantum Dots* **IT-14:** Santosh Gupta, BARC, Mumbai *TBA* **Contributory presentation:** d0018
13:00-14:00	**Lunch Break**	
14:00-16:00	**Session 5: Contributary oral presentation** **Session chair:** Debasis Sen, BARC, Mumbai ***(Venue: Auditorium 1)***	**Session 6: Novel Magnetic Phenomena** **Session Chair:** Aftab Alam, IITB, Mumbai ***(Venue: Auditorium 2)***
	Contributary presentations: c0023, c0063, c0102, d0027, e0012, f0022, f0030, l0006	**IT-15:** Chandan Mazumdar, SINP, Kolkata *Novel Magnetic Phenomena in Quaternary Heusler Alloys* **IT-16**: Ashis Bhattacharjee, Visva-Bharati University, Santiniketan *High Spin ⇄ Low Spin Transition in Iron(II) Complexes:* *Effect of External Stimuli* **IT-17**: Ram J. Choudhary, UGC-DAE CSR, Indore *Electronic Structure Aspects of Tunable Ferromagnetic and Antiferromagnetic States in the Charge Transfer materials: A Case Study of SrCoOx Thin Films* **IT-18:** Anil Jain, BARC, Mumbai

		Exotic Ground States and Spin Dynamics in One-Dimensional and Two-Dimensional Quantum Magnets
16:00-18:00	**Tea and Poster Presentation**	
	a0007 to a0017, b0011 to b0018, c0013 to c0035, d0008 to d0015, e0005 to e0008, f0007 to f0016, g0007 to g0022, h0010 to h0017, i0012 to i0017, j0016to j0028, k0014 to k0031, l0009 to l0015	
18:00-19:30	**Cultural Programs**	
19:30	**Dinner**	

Day 3: Friday, December 20, 2024

9:30-10:10	**Pl 5:** Sean Langridge, ISIS, RAL UK *Applying polarised neutron techniques to the study of topologically nontrivial materials* **Session Chair:** A. Sundaresan, JNCASR Bengaluru **(A1)**	
10:15-11:15	**Session 7: Quantum materials** **Session Chair:** Sean Langridge, ISIS, RAL UK ***(Venue: Auditorium 1)***	**Session 8: Surface and Interface Physics** **Session Chair:** R. Mittal, BARC, Mumbai ***(Venue: Auditorium 2)***
	IT-19: Bhavtosh Bansal, IISER Kolkata *Solid state phase transitions with hysteresis: Mean field universality and beyond* **IT-20:** Arnab Banerjee, Purdue University, USA *Quantum Coarsening Dynamics in Frustrated Magnetic Hamiltonians using Quantum Simulators*	**IT-23**: Gianluca Ciatto, Soleil Synchrotron, France *In situ synchrotron radiation characterisation of the incipient growth of functional materials via atomic/molecular layer deposition* **IT-24:** Karthik V Raman, TIFR(H), Hyderabad *In-Plane Anisotropy of Magnetic Textures Revealed by Planar Hall Effect*
11:15-11:45	**Tea Break**	
11:45-13:00	**Session Chair:** Thamizhavel Arumugam, TIFR, Mumbai	**Session Chair:** G. Ravi Kumar, GITAM, Vizag **IT-25:** Neeraj Khare, IITD, New Delhi

	IT-21: Srimanta Middey, IISC Bengaluru *Engineering collective quantum phenomena in oxide heterostructures* **IT-22:** Sudipta Kanungo, IIT Goa *Tale of Iridates: How strong is the spin orbit coupling in reality* **Contributory presentation:** l0031	*Ferroelectric Films for Clean Energy Generation using Piezo and Tribo Effect* **IT-26:** A. Biswas, BARC, Mumbai *X-ray-based investigations on interface engineered Neutron and X-ray multilayers* **Contributary presentation:** f0048
13:00-14:00	**Lunch Break**	
14:00-16:00	**Session 9: Contributary oral presentation** **Session Chair:** Mala N. Rao, BARC, Mumbai ***(Venue: Auditorium 1)***	**Session 10: Physics of Energy Materials** **Session Chair**: D V Udupa, BARC, Mumbai ***(Venue: Auditorium 2)***
	Contributed Oral Presentations g0004, g0007, h0040, h0051, h0055, d0040, d0031, i0017	**IT-27:** Tanmoy Maiti, IITK, Kanpur *High Performance Thermoelectric Nanocomposites with 2D Graphene and MXene* **IT-28:** Abhik Banerjee, TCG CREST, Kolkata *Developing Safe, Cost Effective and High Energy Density Solid State Battery* **IT-29:** M. Navaneethan, SRM Chennai *Interfacial Engineering for Advanced Wearable and Bulk Thermoelectric Devices* **Contributed Oral Presentations:** d0041, k0008
16:00-18:00	**Tea and Poster Presentations**	
	a0018 to a0027, b0019 to b0024, c0036 to c0056, d0016 to d0022, e0009 to e0015, f0017 to f0028, g0023 to g0034, h0018 to h0028, i0018 to i0025, j0029 to j0045, k0032 to k0050, l0016 to l0022	
18:00-19:00	**Industry Interaction**	
19:30	**Dinner**	

Day 4: Saturday, December 21, 2024

<table>
<tr><td>09:30-10:10</td><td colspan="2">Pl 6: Ravindra Kumar G, TIFR, Mumbai
Extreme States with Ultrahigh Intensity, Ultrafast Laser Pulses- Hot, Dense Matter
Session Chair: T. Sakuntala, BARC, Mumbai
(Venue: Auditorium 1)</td></tr>
<tr><td>10:15-11:00</td><td>Session 11: Thesis Presentations
Session chair: Chandan Mazumdar, SINP, Kolkata
(Venue: Auditorium 1)</td><td>Session 12: Young achiever presentations
Session Chair: K. Maiti, TIFR, Mumbai
(Venue: Auditorium 2)</td></tr>
<tr><td>11:00-11:30</td><td colspan="2">Tea Break</td></tr>
<tr><td>11:30-13:00</td><td>Thesis Presentations (contd.)</td><td>Young achiever presentations (contd.)</td></tr>
<tr><td>13:00-14:00</td><td colspan="2">Lunch Break</td></tr>
<tr><td>14:00-16:00</td><td>Session 13: Dynamics and critical phenomena
Session Chair: K. G. Suresh, IITB, Mumbai
(Venue: Auditorium 1)</td><td>Session 14: Neutron: Probe for condensed matter Physics
Session Chair: P. D. Babu, UGC-DAE CSR, Mumbai
(Venue: Auditorium 2)</td></tr>
<tr><td></td><td>IT-30: Sunil Kumar, IITD
Ultrafast terahertz dynamics in solids and interfaces
IT-31: Gopal Dixit, IITB, Mumbai
IT-32: Boby Joseph, Elettra, Italy
Pressure-induced structural modifications in Remeika phase quasi skutterudite stannides
Contributed Oral Presentations: j0083, i0036</td><td>IT-33: A Sundaresan, JNCASR, Bengaluru
Correlation between magnetic structure and magnetoelectric properties of the green phases R_2BaCuO_5 (R=Rare-earth)
IT-34: Russell Ewings, ISIS, RAL, UK
Entangled orbital, spin and ferroelectric order in cesium superoxide
IT-35: S. D. Kaushik, UGC-DAE CSR, Mumbai
Neutron diffraction: An unambiguous tool for characterizing magnetism in emerging materials
Contributed Oral Presentations: a0004, j0072</td></tr>
<tr><td>16:00-18:00</td><td colspan="2">Tea and Poster Presentation</td></tr>
</table>

	a0028 to a0035, b0025 to b0033, c0057 to c0081, d0023 to d0030, e0016 to e0019, f0029 to f0039, g0035 to g0046, h0029 to h0041, i0026 to i0030, j0046 to j0064, k0051 to k0072, l0023 to l0031
19:30	**Dinner**

Day 5: Sunday, December 22, 2024

9:30-10:10	**L. M. Pant, Single Crystal activities at BARC** **Session chair:** Raghvendra Tewari, BARC, Mumbai ***(Venue: Auditorium 1)***
10:15-11:45	**Session 13: Topological and Multifunctional Materials** ***(Venue: Auditorium 1)*** **Session Chair:** Indranil Das, SINP, Kolkata
	IT-36: B. R. K. Nanda, IITM *Field Tunable band topology and topological Hall effect in skyrmion crystals* **IT-37:** Amit Agarwal, IITK *Hidden Berry curvature and planar Hall effect in 2D materials* **IT-38:** Kamlendra Awasthi, MNIT Jaipur *Polymer nanocomposite membranes for gas separation and sensing*
11:45-13:15	**Tea and Poster Presentations**
	a0036 to a0048, b0034 to b0039, c0082 to c0103, d0031 to d0041, e0020 to e0025, f0040 to f0050, g0047 to g0062, h0042 to h0055, i0031 to i0037, j0065 to j0084, k0073 to k0102, l0032 to l0037
13:15-14:15	**Lunch**
14:15-15:00	**Award Presentations** S. M. Yusuf, BARC Mumbai L. M. Pant, BARC Mumbai ***(Venue: Auditorium 1)***
15:00-15:30	**Concluding Session** **Concluding Remarks:** S. M. Sharma, BARC, Mumbai ***(Venue: Auditorium 1)***

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ABSTRACTS

PLENARY TALKS

PL-1

Designing New Materials for the evolving energy landscape and sustainable development

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Abstract: Internationally the energy landscape is evolving very rapidly with a strong drive towards a significantly enhanced use of clean and renewable energy in the energy mix. It is realized by the scientific community that the Sustainable Development Goals (SDGs) set by UN can be realized over the projected time scales only by rapid advancements in new and affordable clean energy technologies. This necessitates a pragmatic innovation approach based on the use of earth abundant materials, and simplified processing methodologies including energy-saving green processing methods. I will outline this emergent scenario starting from general principles followed by some specific examples derived from own research along these lines in the domain of energy harvesting and storage.

PL-2

Quantum Materials *by* Computation: Challenges & Opportunities

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Abstract: In recent time, there has been a world wide surge of activity on Quantum materials, materials whose properties are dominated by quantum fluctuations, quantum entanglement, quantum coherence, topological behavior. In this talk, I will discuss the contribution of computation in understanding and predicting these materials. In particular, I will discuss its application in understanding materials properties by understanding the structure-property relation, prediction of new functionalities in known materials, and predicting new materials all together.

PL-3

Fragmentation Concepts explain Nanoplastic Formation and Temporal Persistence

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Abstract: Roughly 85% of all polymers are not recycled – much of this waste plastic ends up in the environment. Many wear mechanisms (light, stresses, weathering) lead these materials to form nanoplastics which could have deleterious consequences on human and animal health. We study the mechanism of nanoplastic formation in two canonical cases – rubber tires and semicrystalline polymers (the latter comprise more than 75% of all polymers we use). We show that while nanoplastic formation in the two cases have very different mechanisms, that they are unified by the concept of fragmentation. Both experimental and theoretical aspects of these situations are touched on, and we shall examine mitigation strategies, time permitting.

PL-4

Computational materials science and its applications in the area of materials for energy

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Abstract: Energy storage has been a theme for scientists for two hundred years. The Lead acid battery research on batteries occupied some of the best minds of the 19th century. Gaston Plante in 1859 invented the lead acid battery which starts your car and ignites the internal combustion which takes over the propulsion. Although the lead battery is over 150 years old but the origin of its open circuit voltage (OCV) of 2.1 V is still known. In present talk, I will show how one can explain the origin of OCV of 2.1 V based on foundations of relativistic quantum mechanics. Surprisingly, seems to be the first time its chemistry has been theoretically modelled from the first principles of quantum mechanics. The main message of this work is that most of the electromotoric force (1.7-1.8 Volts out of 2.1 V) of the common lead battery comes from relativistic effects. While the importance of relativistic effects in heavy-element chemistry is well-known since over two decades, this is a striking example on "everyday relativity". We believe that the fact that "cars start due to relativity."
The purpose of this talk is to provide an overview of the most recent studies in the field of hydrogen storage materials & rechargeable battery research with the focus how computational material science can play an important role in search and design of new hydrogen storage materials & next generation battery materials. On specific examples, the application of density functional theory calculations and molecular dynamics simulations

will be illustrated to show how these computational methods can be of great use in the effort to reach a better understanding of materials and to guide the search for new promising candidates.

PL-5

Applying polarised neutron techniques to the study of topologically nontrivial materials

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Abstract: Topologically non-trivial materials remain a central research theme of contemporary condensed matter physics. Topologically protected electronic band structure and spin structures result in a range of emergent phenomena that is of interest at both a basic and applied level. Two examples of such matter are skyrmions, topological swirls of magnetization that have potential for neuromorphic computing1 and magnetic topological insulators that have been shown to exhibit the quantum hall effect2.
To fully understand these materials often requires the application of a broad spectrum of experimental techniques. In this talk we will illustrate how the nanoscale sensitivity of polarised neutron techniques can be applied to the search for proximity polarised topological insulators3 and the dynamic bending of skyrmion tubes4.

1. Huang, Y., Kang, W., Zhang, X., Zhou, Y. & Zhao, W. Magnetic skyrmion-based synaptic devices. *Nanotechnology* **28**, 08LT02 (2017).
2. Chang, C.-Z. *et al.* Experimental Observation of the Quantum Anomalous Hall Effect in a Magnetic Topological Insulator. *Science* (2013) doi:10.1126/science.1234414.
3. Awana, G. *et al.* Critical analysis of proximity-induced magnetism in MnTe/Bi2Te3 heterostructures. *Phys. Rev. Mater.* **6**, 053402 (2022).
4. Ran, K. *et al.* Bending skyrmion strings under two-dimensional thermal gradients. *Nat. Commun.* **15**, 4860 (2024).

PL-6

Extreme States with Ultrahigh Intensity, Ultrafast Laser Pulses- Hot, Dense Matter

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Abstract: Creation of extreme states characterized by high temperature ***simultaneous*** with high density, akin to those in stellar atmospheres, has been made possible by the spectacular advances in high energy, ultrashort laser pulses [1]. The current world record for peak laser power is 10 petawatt and focused intensities attainable with such pulses have already reached 10^{23} Wcm^{-2}. In this talk, we will look at some of the work performed by the TIFR 150 terawatt, 30 femtosecond laser that can attain peak intensities close to 10^{20} W cm^{-2}. The femtosecond, relativistic electron pulses that are created in a solid at such laser intensities dominate the ultrafast dynamics in the generated hot, dense matter, manifesting giant magnetic fields [2,3], ultrahard x-ray emission, fast ion generation etc. [1] The processes are of interest to condensed matter science and technologies, in terms of the gigantic pressures achieved [1] shocks [4,5] that induce dramatic phase transformations [6], large scale ordering of spin structures and magnetic domains and 'hot' solid physics. We highlight the crucial role of nanoscience in the generation of such extremes [1]. I will describe the results of our experiments and simulations after an introduction to the subject area.

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References:

1. J. J. Rocca et al, OPTICA, **11,** 437 (2024)
2. G. Chatterjee et al., Phys.Rev.Lett. **108**, 235005 (2012)
3 G. Chatterjee et al., Nature Commun. 10.1038/NCOMMS15970 (2017)
4. S. Mondal et al., Phys. Rev. Lett. **105**, 105002 (2010); A. Adak et al, Phys. Rev. Lett **114**, 115001 (2015)
5. K. Jana et al., Phys Rev Res. **3**, 033304(2021)
6. A. Bisht et al., Acta Materialia **150**, 161 (2018)
7. K. Nath et al, New J. Phys. **23**, 083027 (2021); J. Sinha et al, Phys. Rev. **E 77**, 046118 (2008)

EVENING TALK

ET-1

Intersection – Physics & AI

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Abstract: The intersection of AI and physics represents unfolding of an exciting frontier in science. The synergy between these fields is driving new discoveries and enhancing research methodologies leading the way for technological innovations. The collaboration between AI and physics promises to shape the future of scientific research and our understanding of the universe. This interdisciplinary field is unlocking groundbreaking possibilities, from accelerating scientific research to developing cutting-edge applications We shall a begin by touching upon convergence of the two fields which has led to recognition by Nobel prize. Some of the things we shall also address are

1. Machine Learning for Physics:

o **Data Analysis and Pattern Recognition:** AI algorithms are adept at analyzing vast datasets generated by experiments and simulations, uncovering hidden patterns and correlations.

o **Accelerating Simulations:** AI-powered techniques can significantly speed up complex physical simulations, enabling researchers to explore a wider range of scenarios.

o **Predictive Modeling:** AI models can make accurate predictions about the behavior of physical systems, aiding in forecasting and decision-making.

2. Physics-Inspired AI:

o **Neural Networks:** Inspired by the structure of the human brain, neural networks are a cornerstone of AI. They are used to model complex systems and learn from data.

Quantum AI: Quantum mechanics is being harnessed to develop quantum computers, which have the potential to revolutionize AI by solving problems that are intractable for classical computers.

SPECIAL LECTURE

SL-1

Single Crystal activities at BARC

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Abstract: Single crystals play a crucial role in a wide range of advanced technologies, with nuclear radiation detection being one of their key applications. The development of effective radiation detectors relies on the growth of large single crystals with specific desired properties. At BARC, the crystal growth facility specializes in producing large single crystals, primarily for use in nuclear radiation detectors, through melt growth techniques. This presentation will highlight the expertise developed in growing single crystals of various halide and oxide materials, along with the advancements in detector development. Additionally, ongoing research into cutting-edge materials will be discussed, along with a forward-looking roadmap, including plans to establish a unique crystal growth center at BARC VIZAG.

INVITED TALKS

IT-1

Spin-1/2 kagome Heisenberg antiferromagnet: New insights from Machine Learning approaches

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Abstract: The ground state of S=1/2 Heisenberg antiferromagnet on the kagome lattice is one of the most widely studied paradigmatic models of a quantum spin liquid. However, despite numerous studies using both analytical and numerical approaches, the true nature of the ground state and low- energy excitations in this system remain debated. This is related to the difficulty in determining the spin gap in various calculations. We present the results of our investigation of the Kagome AFM using the recently developed group equivariant convolutional neural networks – an advanced machine learning technique for studying strongly frustrated models. The approach, combined with variational Monte Carlo, introduces significant improvement of the achievable results accuracy in comparison with approaches based on other neural network architectures that lack generalization quality for frustrated spin systems. Our results strongly indicate that the ground state of the kagome lattice antiferromagnet is a spinon pair density wave that does not break time- reversal symmetry or any of the lattice symmetries. The found state appears due to the spinon Cooper pairing instability close to two Dirac points in the spinon energy spectrum and resembles the pair density wave state studied previously in the context of underdoped cuprate superconductors in connection with the pseudogap phase. The state has significantly lower energy than the lowest energy states found by the SU(2) symmetric density matrix renormalization group calculations and other methods.
Ref.: Tanja Đurić, Jia Hui Chung, Bo Yang, and Pinaki Sengupta, "Spin-1/2 kagome Heisenberg antiferromagnet: Machine learning discovery of the spinon pair density wave ground state", arXiv:2401.02866 (2024).

IT-2

Magnetic-field free switching of ferromagnetic layers through Interfacial engineering

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The ability to control and switch magnetization via current-induced torque offers significant advantages in reduced power consumption for memory devices and spin logic applications. In a system composed of heavy metal (HM) / ferromagnet (FM) / heavy metal (HM) possessing perpendicular magnetic anisotropy with broken normal space inversion symmetry (SIA), the current-induced magnetization reversal (CIMR) is facilitated by spin-orbit torque (SOT), typically requiring the assistance of an in-plane magnetic field. Conversely, in an HM/FM/HM-based system with broken lateral symmetry, known as a quasi-PMA system, CIMR can occur without such assistance, emphasizing its importance in achieving magnetic field-free CIMR. The spin-orbit torque arises from the spin-Hall effect and the Rashba effect, which are both consequences of SIA. Here, I present three case studies highlighting the vital role of interfacial engineering in fine-tuning CIMR and achieving magnetic field-free switching. In the first case study, field-induced domain wall motion was analyzed to determine the Dzyaloshinskii-Moriya interaction strength (D_{eff}) in Ta/Pt/Co/Au(t)/Pt multilayers with Au layer thicknesses (t) of 0, 0.3, 0.5, and 0.7 nm. The domain wall chirality was inferred from the asymmetric expansion of bubble domains within the system. The second case study involves modifying the bottom Pt/Co interface in Ta/Pt/Co/Pt-based PMA systems by incorporating a 1 nm Au layer, effectively reducing the critical current density (J_c). Micromagnetic simulations provided qualitative estimates of the spin-Hall angle (θ_{sh}). Furthermore, field-free switching at a reduced J_c was achieved using interlayer exchange coupling between perpendicularly magnetized and in-plane magnetized Co layers, mediated by a Ta layer. The third case study focuses on the Pt/Co/Pt multilayers deposited on Ta and Ta/Cu layers, aiming to investigate current-induced magnetization reversal and evaluate J_c. The Cu layer's orbital current enhanced the effective θ_{sh} of the system and reduced J_c. Notably, field-free switching was observed exclusively in Ta/Cu/Pt/Co/Pt multilayers with Cu layer thicknesses of 2 and 4 nm. Micromagnetic simulations confirmed the emergence of additional spin polarization along the z-direction, supplementing the traditional y-direction spin polarization induced by the spin-Hall effect, thus supporting field-free switching. These case studies collectively underscore the strategic importance of interfacial engineering in optimizing CIMR and enabling magnetic field-free switching, paving the way for advanced applications in spintronic devices.
*In collaboration with Saikat Maji

IT-3

Novel Magnetic & Electrical Transport in Non-coplanar Magnetic Textures

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Abstract: The realization of non-centrosymmetric magnetic Weyl metals is anticipated to yield unique anomalous transport properties arising from the interplay between bulk electronic topology and complex magnetic structures. In this talk, we present the discovery of a rare spin-valve-like magnetoresistance at room temperature in the bulk ferromagnetic Weyl metal Mn_2PdSn, which crystallizes in the inverse Heusler (iHA) structure. This system exhibits a substantial anomalous Hall conductivity (AHC) mediated by intrinsic Weyl nodes. A simple substitution of tin with indium leads to the emergence of a double-spin-glassy transition, though the origin of the AHC remains unchanged. Further chemical tuning, achieved by replacing half of the palladium atoms with Iridium to form $Mn_2Pd_{0.5}Ir_{0.5}Sn$ in a tetragonal D_{2d} structure, introduces the conditions required for the stabilization of an anti-skyrmion phase. This transformation results in a giant topological Hall effect, alongside the presence of 42 Weyl node pairs near the Fermi surface, contributing to a significant intrinsic AHC. The talk will conclude with a discussion on the simultaneous realization of topological electronic band structures with magnetic phases in correlated polar magnets and investigation of critical behavior employing AHC, highlighting the potential to leverage novel quantum functionalities.

Reference:

1. Spin-valve-like magnetoresistance and anomalous Hall effect in magnetic Weyl metal Mn_2PdSn. - *Arnab Bhattacharya, et al.* **Phys. Rev. B 110, 014417 (2024)**
2. Critical behavior and phase diagram of skyrmion-hosting material Co3.6Fe4.4Zn8Mn4 probed by anomalous Hall effect. – *Ahmed et al.* **J Alloys Compds 960, 170274 (2024)**
3. Giant Topological Hall Effect in Magnetic Weyl Metal Mn2Pd0.5Ir0.5Sn - *Arnab Bhattacharya, et al* **arXiv: 2410.15011**

IT-4

Exploring the structural contribution to dynamics in supercooled liquids

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Abstract: The behaviour of supercooled liquid differs significantly from that of the normal liquid. While the dynamics undergo significant changes, the structure only exhibits marginal change. The origin of dynamic heterogeneity (DH) in supercooled liquids is a subject of intense research. It is often theorised that, similar to crystals, structural defects exist in supercooled liquids, leading to DH. However, pinpointing structural defects in a supercooled liquid is a challenging task. In this presentation, I will introduce a newly proposed order parameter, the softness of a mean-field caging potential, described in terms of pair structure, and demonstrate that i) the overall dynamics of the system can be described using the average softness parameter and ii) the local dynamics is causally related to the local structure in the supercooled regime, where a separation between short and long time dynamics occurs, enabling a static description of the cage. Using this structural metric, I will then illustrate how the correlation between structure and dynamics can be employed to investigate various phenomena, such as differences in dynamics in systems interacting via attractive and repulsive potentials. Lastly, I will discuss a recent study that showcases the utility of this structural metric in experimental colloidal systems for characterising local structural heterogeneity and its connection to dynamics in both quiescent and sheared systems.

REFERENCES

[1] M. K. Nandi, A. Banerjee, C. Dasgupta and S.M. Bhattacharyya Phys. Rev. Lett., **119**, 265502 (2017)
[2] M. K. Nandi and S. M. Bhattacharyya, Phys. Rev. Lett.**126**, 208001 (2021).
[3] M. Sharma, M. K. Nandi, S. M. Bhattacharyya, Phys. Rev. E **105**, 044604 (2022). [4] M. Sharma, M. K. Nandi and S. M. Bhattacharyya, J. Chem Phys, **159**, 104502 (2023)
[5] R. Sahu, M. Sharma, P. Schall, S. M. Bhattacharyya, V. Chikkadi, PNAS **121** (42) e2405515121 (2024).

IT-5

Crafting Perfection: Annealing a Granular Polycrystal

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Abstract: Disks of equal size should readily fit together to form a crystal. In reality, it happens very infrequently! Any minor hiccup, particularly from friction, can disrupt the neat order, leaving us with an arrangement of polycrystals. It would be interesting to know how to anneal such polycrystals into a single crystal. In this talk, I will demonstrate how this can be achieved. Under the effect of oscillatory shear, a monolayer of frictional granular disks can undergo two phase transitions: a transition from an initially disordered state to an ordered crystalline form, and a dynamic active-absorbing phase transition. Although there is no obvious reason for them to be at the same critical point, they are. The transitions may also be characterized by the disk trajectories, which are nontrivial loops breaking time-reversal invariance.

IT-6

Beyond Brownian Motion: Non-Markovian and Non-Gaussian Mechanisms of Molecular Diffusion in Complex Fluids

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Abstract: For over a century, the concept of Brownian motion has been fundamental to describing diffusion in fluids, predicated on the assumptions of Markovianity and Gaussianity. While these assumptions hold in many systems, advances in experimental and simulation methodologies now allow us to scrutinize their validity more critically. This talk delves into various complex fluids that exhibit significant deviations from Brownian motion, presenting comprehensive theoretical models and experimental results that highlight non-Gaussian and non-Markovian diffusion mechanisms. While studying lipid lateral diffusion within membranes, we observed subdiffusive behavior characterized by non-Markovian dynamics and a power-law memory function [1]. Interestingly, despite the subdiffusion, the process follows a Gaussian approximation, with subdiffusion linked to medium-induced viscoelasticity. Meanwhile, in deep eutectic solvents (DESs), QENS experiments reveal non-Gaussian molecular diffusion [2]. MD simulations indicate that this is due to a cage-jump diffusion mechanism, where molecular caging is associated with complex formation [3]. Through extensive modeling based on a non-local diffusion equation, which is entirely Markovian in nature, we elucidate how the jump diffusion process leads to non-Gaussian diffusion mechanism [4]. Lastly, systems exhibiting both non-Markovian and non-Gaussian behaviors simultaneously will be discussed. The phenomenon of sub-diffusion crossover in glass-forming liquids exemplifies this, necessitating such a dual consideration [5]. The diffusion process in these systems is effectively modeled using non-Gaussian fractional Brownian motion (nGfBm), which successfully explains QENS data for various molecular and polymeric glass-formers. In this talk, we explore the potential of extending diffusion models to incorporate non-Gaussian and non-Markovian effects by augmenting the Brownian model [6] using non-local diffusion equations with insights from QENS experimental investigations and MD simulations.

References:

[1] H. Srinivasan, V. K. Sharma, S. Mitra and R. Mukhopadhyay, *J. Phys. Chem. C* 122, **2018**, 20419
[2] H. Srinivasan, V. K. Sharma, V. García Sakai, Jan P. Embs, R. Mukhopadhyay and S. Mitra, *J. Phys. Chem. B* 124, **2020**, 1509
[3] H. Srinivasan, V. K. Sharma, R. Mukhopadhyay and S. Mitra, *J. Chem. Phys.* 153, **2020**, 104505
[4] H. Srinivasan, V. K. Sharma, V. García Sakai, R. Mukhopadhyay and S. Mitra, *J. Phys. Chem. Lett.* 14, **2023**, 9766
[5] H. Srinivasan, V. K. Sharma, V. García Sakai and S. Mitra, *Phys. Rev. Lett.* 132, **2024**, 058202
[6] H. Srinivasan, V. K. Sharma and S. Mitra, *Phys. Chem. Chem. Phys.* **2024** (in press; DOI:doi.org/10.1039/D4CP01813C)

IT-7

Accelerating the Discovery of Ambient-Pressure High-Temperature Superconductors through Ab-initio Structure Search and Machine Learning

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The discovery of high-temperature superconductors suitable for practical applications remains a central challenge in materials science, particularly at ambient pressures. Hydrogen-rich materials have long been explored for their potential to support conventional phonon-mediated superconductivity; however, their application is often limited by the extreme pressures required for stability. Here, we present a high-throughput computational approach to identify promising superconductors within a broad composition space of high-symmetry ternary hydrides from across the periodic table, specifically focusing on materials stable at ambient pressure. Through a workflow integrating ab-initio random structure search (AIRSS), machine learning (ML), and density functional perturbation theory (DFPT), we efficiently narrowed the candidate pool based on thermodynamic, dynamic, and magnetic stability considerations before directly estimating superconducting critical temperatures.

This approach has revealed a metastable ambient-pressure hydride superconductor, Mg_2IrH_6, with a predicted critical temperature of 160 K [1], comparable to the highest temperature superconducting cuprates. We propose a synthesis route via a structurally related insulator, Mg_2IrH_7, which is thermodynamically stable above 15 GPa, and discuss the potential challenges involved. Experimental efforts have also been made to synthesize the superconducting Mg_2IrH_6 via another insulating phase, Mg_2IrH_5 [2].

References

[1] K. Dolui, L.J. Conway, C. Heil, T.A. Strobel, R. Prasankumar, C.J. Pickard, Phys. Rev. Lett. 132, 16601 (2024).
[2] Mads F. Hansen et al. Preprint at arXiv:2406.09538; accepted in Phys. Rev. B (2024).

IT-8

Uncovering Multifold Phonon Degeneracies in Cubic Nb_3Bi

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Abstract: Topological materials are of considerable interest due to their unique properties and promising applications. Topological states with multifold band degeneracies extend beyond electronic systems to include phononic systems as well. In this study, we explore the higher-order symmetry-enforced topological characteristics of Nb_3Bi, an intermetallic compound with an A15 crystal structure. Using first-principles calculations and symmetry analysis, we characterize the topological phonon modes protected by nonsymmorphic symmetries. Our findings reveal significant degeneracies in the phonon dispersion relations of Nb_3Bi, most notably a sixfold degenerate point located at the R point of the Brillouin zone. Additionally, we identify cubic Dirac contact points and quadratic triple points at the R and Γ points, respectively. Phonon surface state calculations on two different terminations, (001) and (110), exhibit distinct twofold rotational symmetry patterns. These results provide valuable insights into the unique phononic features and surface states of Nb_3Bi, underscoring its potential significance in the study of topological phonons.

IT-9

Polarization Coupled Magnetization Switching in ABO_3 Oxides

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Abstract: A key criterion for multiferroic materials is the ability to achieve combined switching of polarization and magnetization. This can be facilitated by inherent structural distortions and their coupling. In this talk, I will present two examples that demonstrate how structural modes play a crucial role in controlling polarization-magnetization switching. First [1], I will discuss an improper ferroelectric hexagonal ABO_3 system, specifically $Lu_{1-x}Hf_xFeO_3$ (h-LHFO), where heavy electron doping in $LuFeO_3$ (h-LFO) induces spin-disproportionation in the Fe sublattices. Particularly for x = 1/2 and 2/3, this results in robust, room-temperature, out-of-plane, collinear ferrimagnetism, stabilized by a Jahn–Teller metal-to-insulator transition. Additionally, I will present heterostructures combining h-LHFO with a ferroelectric/ferromagnetic (FE/FM) monolayer MnSTe (h-2D), where skyrmions are stabilized without an external magnetic field. The chirality of these skyrmions is controlled by an external electric field via the polarization of h-LHFO, opening new possibilities for magnetoelectric applications.

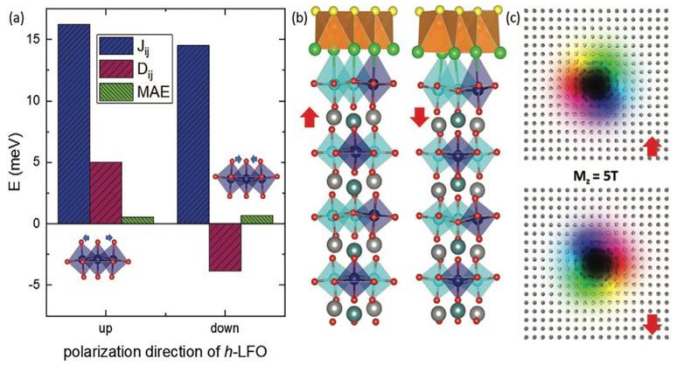

Figure: Polarization - Magnetization Coupling in electron doped h-LHFO

In the second example [2], I will highlight a hybrid improper ferroelectric $AA'FeMoO_6$ double perovskite oxide, where polarization reversal enables switching of the weak magnetization component in a noncollinear $F_xA_yG_z$ configuration. In this system, the primary order parameters are the rotation and tilt of BO_6 octahedra, with A/A' cation ordering facilitating the polarization. We demonstrate that a specific structural distortion, termed "tilt precision," is responsible for the polarization-magnetization coupling.

Acknowledgments
S.G acknowledges SERB Core Research Grant CRG/2023/3209 for funding

References:

[1] M. J. Swamynadhan, Andrew O'Hara, Saurabh Ghosh*, and Sokrates T. Pantelides. Engineering Collinear Magnetization in Hexagonal $LuFeO_3$ and Magnetoelectric Control of Skyrmions in Hexagonal 2D Epilayers, *Adv. Funct. Mater*. 2400195 (2024)
[2] Palanichamy Gayathri and Saurabh Ghosh*, Polarization-Magnetization Switching in a Hybrid Improper Ferroelectric Double Perovskite Oxide above Room Temperature, 2024 (in preparation)

IT-10

The Non-Trivial Topological Landscape of 4D Transition Metal Systems

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Abstract*:* In this presentation, I will discuss the detailed electronic, magnetic, and dynamical properties of 4D transition metal compounds based on our theoretical results. For the first time, we have predicted the non-trivial topological properties of Yttrium Iodide (YI), revealing a unique electronic structure that combines spin-polarized Dirac and Weyl nodes within the same phase. Our study identifies twenty-five pairs of nodal points in the spin-up channel and six pairs in the spin-down channel. The existence of Weyl nodes is confirmed by the source and sink features in the Berry curvature plot and the presence of Fermi arcs in the surface band structure, categorizing YI as a type-II magnetic Weyl semimetal. Under spin-orbit coupling (SOC), eight pairs of Weyl points exhibit robust behaviour, while a small band gap forms at the spin-polarized Dirac cone. The system also demonstrates a high Fermi velocity for Dirac fermions, estimated at 3.4 x 10^5 m/s, and a significant anisotropic intrinsic anomalous Hall conductivity of up to 933 S/cm. The non-trivial topological behaviour of ZrN will also be discussed, in which Dirac nodal line semimetallic behaviour is recently predicted through our investigation. The non-trivial properties such as Weyl points, Dirac points, high intrinsic quantum anomalous Hall conductivity, and Weyl points separated by long distances in momentum space make these materials highly potential for spintronic applications.

IT-11

Phonons at nanoscale

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Abstract: Confinement of both acoustic and optical phonons at micro- and nanoscale was a hot topic at the end of last century with a remanence till the beginning of this century. The confined acoustic phonon was studied for non-destructive characterization of both the size and shape of tiny matter. Confinement of optical phonon, on the other hand, was used to understand the shape of phonon mode and analyze stress in material combing shift in the mode frequency. Interface phonons was also discussed during this time period, where surface modes were probed to characterize both interface structure and surface morphologies in nanomaterials. All these studies were part of far-field optics. However, near-field optics have started dominating the present century with the application of surface plasmon resonance using noble metal nanostructures. The spectroscopic study in the near-field became a potential technique for studying the properties of nanostructures without the use of nano-manipulator. Optical microscope-based conventional techniques, however, are limited by sub-diffraction limits. Plasmon is a collective oscillation of conduction electrons that helps electromagnetic waves behave differently and in an evanescent way. The latter makes the light to find objects which are far beyond its reach. In this regard, plasmon assisted tip enhanced Raman spectroscopic (TERS) studies of the semiconducting system are made the nanoscale. A localized study of the quantum-confined 0D SnO_2 was reported [1]. A doping study in 1D GaN nanowire was reported [2]. The electronic effect on the phonon characteristic of single Si nanowire [3], 2D-MoS_2 [4], and bilayer V_2O_5 [5] are also discussed [3,4]. Low frequency Bosonic mode is also probed in characterizing spinon vibration in 1D spin ½ Heisenberg chain of VO_2 [6].

References:

[1] B. Venkataraman, A. Das , A. K. Sivadasan, A. K. Tyagi, S. Dhara, *J. Raman Spectrosc.* [Rapid Commun.] **46** (2015) 1037.
[2] A. Patsha, S. Dhara, and A. K. Tyagi, *Appl. Phys. Lett.* **107** (2015) 123108.
[3] A. Patsha, and S. Dhara, *Nano Lett.* **18** (2018) 7181.
[4] K. K. Madapu, C. Abinash Bhuyan, S. Dhara**,** *Phys. Rev. B* **108** (2023) 085429.
[5] P. R. Reshma, P. Anees, S. Sinha, A. Dasgupta, K. Ganesan, A. K. Prasad, **S. Dhara** *J. Phys. Chem. Lett.* **12** (2021) 9821
[6] R. Basu, V. Srihari, M. Sardar, S. Srivastava, S. Bera, S. Dhara, *Sci. Rep.* **10** (2020) 1977.

IT-12

Two-dimensional materials for next-generation electronics and optoelectronics technologies

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Abstract: Atomically-thin materials possess unique intrinsic properties and are amenable to a range of tuning techniques. We harness these properties underpinned by application demand and work with industry to translate

into end-user products. Firstly, we synthesise a variety of atomically-thin metal oxides, mono/dichalcogenides and elemental 2D materials using solid, liquid and vapour phase techniques guided by application. Our fundamental advances have been uncovering the origins of oxidative degradation in few-layer black phosphorus (BP) and subsequently proposing an ionic liquid-based approach to prevent ambient degradation of BP. Using defect engineering, we have demonstrated neuromorphic vision and processing sensors. We have explored the use of hybrids of dissimilar materials to enhance electronic and optical performance. Ultra-thin layers have been used to develop one of the world's thinnest photodetectors that can sense all shades of light from UV-infrared. We further study strain-tunability in low-dimensional structures via integrating them onto elastomeric platforms.
Recently, we have investigated the influence of defects and strategies for passivation in monolayer transition metal dichalcogenides for applications in optoelectronics and health sensors. Using a cross-disciplinary approach, we deploy multifunctionality of these new material systems into solving technological challenges for industry partners across sectors that require novel materials and functions to be integrated into their products.

IT-13

Efficiency enhancement of the Organic Photo Voltaic Cells through the doping of nano materials in the discotic liquid crystals

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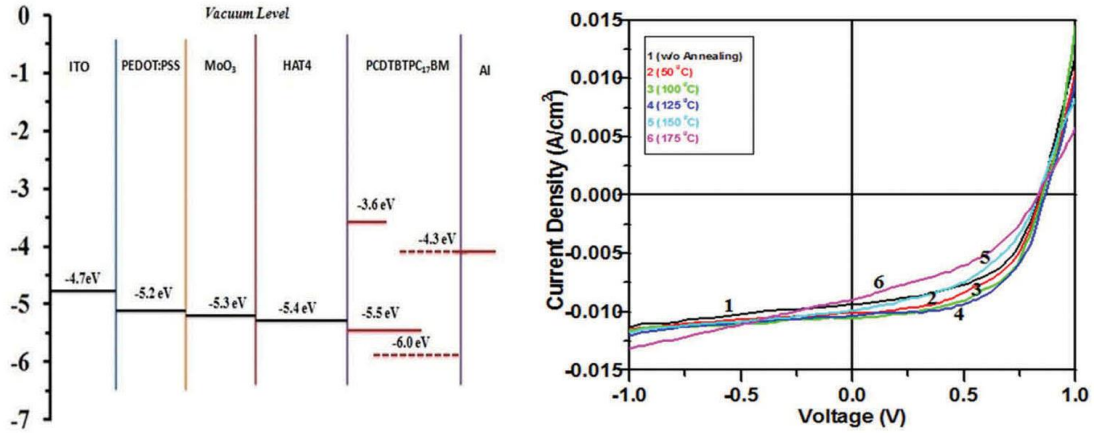
Abstract: Discotic liquid crystalline (DLC) materials with dopped nano entities have very good prospect to be used in flexible Photovoltaic/Solar cells [1]. Cells based on composites of copolymer poly [N-90-heptadecanyl-2,7-carbazole-alt-5,5-(40,70-di-2-thienyl-20,10,30-benzothiadiazole)] and the fullerene derivative [6,6]- phenyl C71-butyric acid methyl ester with a layer of DLC material (2, 3, 6, 7, 10, 11-hexabutyloxytriphenylene) between the interface of active layer and hole transporting layer will be discussed.



Different hole transporting layers deposited on indium tin oxide substrates such as poly (3,4-ethylenedioxythiophene)-poly (styrene sulphonate) or molybdenum trioxide have been used in these devices. The influence of varying the thickness of liquid crystal layer and annealing on the photovoltaic parameters of these devices was studied. All the devices with inserted DLC layer show better performance than the reference cells. Power conversion efficiency >5% was achieved for the solar cells containing self-organized DLC layer of 30 nm thickness under one sun condition which is substantial jump as compared to earlier reports. The mobility of holes in the DLC inserted devices was found to be ~10^{-6} cm^2 V^{-1} s^{-1} due to which high values of current density was achieved. We target to further enhance the efficiency with appropriate nano structures in the DLCs [2].

References:

1. N. Yadav, R. Dhar, Liquid crystalline materials for efficient solar energy harvesting, p. 211-237 in Unconventional Liquid Crystals and Their Applications, De Gruyter GmbH Berlin, 2021. https://doi.org/10.1515/9783110584370-004
2. A. Khare, R. Uttam, S. Kumar, R. Dhar, Nanocomposite system of a discotic liquid crystal doped with thiol capped gold nanoparticles, J. Mol. Liq. 366, 120215, 2022.

IT-14

The Nobel Prize in Chemistry 2023: Discovery and Synthesis of Quantum Dots

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IT-15

Novel Magnetic Phenomena in Quaternary Heusler Alloys

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Abstract: Quaternary Heusler alloys have garnered significant attention due to their unique electronic and magnetic properties, making them highly promising for a range of technological applications, including spintronics, magnetic sensors, quantum computing, and energy-efficient memory devices. Their tunable half-metallic nature, high spin-polarization, and diverse magnetic states offer potential for creating spin based logic and data storage devices with enhanced performance and reduced power consumption. In this context, understanding the interplay between structural disorder, half-metallicity, and magnetic frustration is vital for harnessing these materials' full capabilities.

In this work, we explore some of the complex behavior of quaternary Heusler alloys, revealing how structural disorder influences their electronic and magnetic properties, often in surprising ways. For instance, in FeMnVZ (Z = Al, Ga) [1,2] compounds, we found robust half-metallic ferromagnetic behavior despite significant crystalline disorder. This resilience of high spin-polarization highlights the potential of these materials for reliable spintronic applications. CoMnCrGa [3], another noteworthy alloy, maintains a half-metallic ferromagnetic state with a high Curie temperature even under structural disorder, making it suitable for room-temperature spintronic devices. The research also uncovers

intriguing magnetic phenomena, such as reentrant spin-glass states in NiRuMnSn [4], where partial disorder leads to magnetic frustration and a transition from weak ferromagnetism to a spin-glass phase. Even more remarkable is FeRuMnGa [5], which, despite its highly disordered and equiatomic structure, stabilizes a pure spin-glass state—a rare occurrence among quaternary Heusler alloys. This unique state is coupled with semi-metallic transport properties and an anomalous Hall effect at low temperatures, illustrating the profound impact of disorder on magnetic and electronic behaviors. Overall, this work provides critical insights into the role of structural disorder in tailoring the magnetic and electronic properties of quaternary Heusler alloys. By revealing novel magnetic states and highlighting the robust half-metallic behavior in disordered systems, this research opens new pathways for the design of advanced materials aimed at next-generation spintronic applications, high-performance magnetic sensors, and energy-efficient quantum devices.

References:

1. S. Gupta *et al*., *Phys. Rev*. B 106, 115148 (2022).
2. S. Gupta *et al*., *Phys. Rev*. B 108, 045137 (2023).
3. S. Gupta *et al*., *J. Mater. Chem.* C, 11, 15489-15499 (2023).
4. S. Gupta *et al*., *Phys. Rev*. B 108, 054405 (2023).
5. S. Gupta *et al*., *Phys. Rev*. B 107, 184408 (2023).

IT-16

High Spin ⇄ Low Spin Transition in Iron(II) Complexes: Effect of External Stimuli

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Abstract: Spin transition (ST) or spin crossover (SCO) is an intrinsic property of all transition metal ions with d^4 to d^7 electronic configurations in octahedral crystal field symmetry of coordination complexes [1-3]. These materials continue to be of great interest in fundamental studies of crystal engineering [4], as components in switching multifunctional materials [5], and for their device applications [6]. The course of the ST in solid materials is influenced by the cooperative interactions between the spin-changing molecules. The cooperativity results from the large difference in the metal-donor atom bond lengths in the two spin states, and it is the measure of the degree of efficiency in the allowance of the intramolecular changes throughout the crystal. For cooperativity to take place, the solid lattice provides the mechanism of communication between the different metal centres. Bridging ligands play important role in influencing this mechanism. Existence of hydrogen bonding interactions too modulates the cooperativity and influences the ST behaviour. ST can be observed by a change in temperature,

pressure and light irradiation [1]. In a thermally-induced spin transition, the LS state will be favoured at low temperatures, whereas at elevated temperatures the HS state will generally occur. In contrast, an increase in pressure usually favours a HS → LS transition. On the other hand, iron complexes exhibit light induced LS ⇆ HS transitions through the LIESST (*light-induced excited spin state trapping*) effect, with green light causing the LS ground state to form a long-lived metastable HS state, and with red light causing it to switch back to the LS state. A large number of iron(II) compounds exhibit low spin (LS, $^1A_1$, $S = 0$) ⇄ high spin (HS, $^5T_2$, $S = 2$) transition under the influence of external perturbations such as temperature, pressure and light. Presently, we will explore the effect of temperature, irradiation of light and application of external mechanical pressure on the spin transition behaviour in $[Fe(bpp)_2](NCS)_2.2H_2O$, (bpp = 2,6-bis(pyrazol-3-yl) pyridine).

Reference:
1. Topics in Current Chemistry; Gütlich, P., Goodwin, H.A., (Eds.) Springer-Verlag: Berlin (2004) Vol. 233-235.
2. Halcrow, M. A., Ed. Spin-Crossover Materials - Properties and Applications; John Wiley & Sons, Ltd.: New York (2013) p 568.
3. Brooker, S., Spin Crossover with Thermal Hysteresis: Practicalities and Lessons Learnt. Chem. Soc. Rev. (2015) 44, 2880.
4. Sugiyarto, K. H.; et al., Cryst Eng Comm (2021) 23, 2854.
5. Wang, M., et al., Coord. Chem. Rev. (2021) 435, No. 213819
6. Molnár, G., et al., Adv. Mater. (2018) 30, No. 1703862.

IT-17

Electronic Structure Aspects of Tunable Ferromagnetic and Antiferromagnetic States in the Charge Transfer materials: A Case Study of $SrCoO_x$ Thin Films

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Abstract: The Metal-insulator transition (MIT) in $SrCoO_x$ (x =2.5 & 3) systems, via electrochemical reaction, is attributed as a Mott-transition, which has tremendous prospects in the new branch of physics called the Mottronic. The reversible switching between the insulating $SrCoO_{2.5}$ and the metallic $SrCoO_3$ phases can be achieved via very small electric bias. To improve the functionality of these devices it is crucial to understand the electronic structure across the different switching states in insulating and metallic regions of the constituent materials. In this framework, our group has recently explored different regions of the Zaanen−Sawatzky−Allen (ZSA)-diagram by varying electronic correlation parameters in $SrCoO_x$ by varying strain in its thin film form. For instance, bulk $SrCoO_{2.5}$ is in the insulating positive charge transfer energy (Δ) regime in the ZSA-diagram and is an antiferromagnetic-insulator. However, by strain engineering, $SrCoO_{2.5}$ thin films move into the insulating negative Δ regime and become ferromagnetic-insulator. On the other hand, oxygen intercalation in $SrCoO_3$ systems (both bulk and thin films) induce a transition into metallic negative Δ regime and become a ferromagnetic-metal. Interestingly, $SrCoO_{2.5}$ can be reversely converted to $SrCoO_3$ by electric biasing also in an all oxide heterostructure, leading to colossal volto-magnetic effect. With these examples, we demonstrate that electronic functionality of $SrCoO_x$ systems can be largely modulated by strain, redox reaction or electric biasing, showing a big potential for Mottronic devices.

IT-18

Exotic Ground States and Spin Dynamics in One-Dimensional and Two-Dimensional Quantum Magnets

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Low-dimensional quantum magnets exhibit a rich tapestry of emergent phenomena driven by enhanced quantum fluctuations and geometric frustration. This talk will explore the magnetic and structural properties of one-dimensional (1D) spin chains and two-dimensional (2D) frustrated lattices, as revealed by neutron and x-ray scattering techniques.

I will first discuss spin-chain systems, emphasizing their exotic ground states and dynamic behaviour. Then, I will shift focus to spin-1/2 kagome compounds, where strong quantum fluctuations and frustration suppress long-range magnetic order, stabilizing novel quantum phases at low temperatures. Results from resonant x-ray scattering and neutron diffraction experiments will illuminate the interplay between spin, lattice, and orbital degrees of freedom in these systems. These studies underscore the pivotal role of advanced scattering techniques in unravelling the physics of quantum magnets, providing a deeper understanding of their complex behaviours and emergent quantum states.

Ref:

[1]. Phys. Rev . B. 110, 224415 (2024).

[2]. Phys. Rev. Mat. 8, 12504 (2024).
[3]. Phys. Rev. B 109, 219903 (2024).
[4]. Phys. Rev. B 107 107, 184406 (2023).
[5]. Phys. Rev. B 108, 174420 (2023)
[6]. Nature Communications 14, 2857 (2023).
[7]. Nature Communications 13, 7665 (2022).
[8]. Chem.Eur.J. ,30,e202303718 (2024)
[9]. Nat. Phys. 13, 633 (2017).
[10]. Phys. Rev. Lett. 123, 137204 (2019).
[11]. Phys. Rev. B (Rapid Comm.) 101, 140413 (2020).
[12]. Phys. Rev. B 102, 134433 (2020).
[13]. Phys. Rev. B 102, 144432 (2020).
[14]. Phys. Rev. Research 2, 043329 (2020).
[15]. Phys. Rev. B 104, 184402 (2021).

IT-19

Solid state phase transitions with hysteresis: Mean field universality and beyond

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Abstract: Many thermally-driven abrupt structural transitions in solid-state systems are observed to be always hysteretic [1]. Based on the understanding gained primarily from the study of the phase transitions in the transition metal oxides (V_2O_3, VO_2, and $NdNiO_3$) and halide perovskites ($MAPbX_3$), I will argue that these must be distinguished from the usual first-order transitions on the account of long-range interactions.
We have observed slowing down of the order parameter fluctuations accompanied by their enhanced variance (`critical opalescence'), and dynamic scaling around the phase transition in these systems [2]. These features which are associated with second-order transitions suggest that the abrupt transition is controlled by a critical-like singularity. The singularities are identified with the spinodal points and vindicate Van der Waals' original mean-field theory for the phase transitions, without Maxwell's correction. I will also describe observations beyond the mean-field scenario, emphasizing the athermal and disorder landscape aspects of these transitions. The ability of these materials to hierarchically encode a large number of metastable configurations via their thermal history and their possible use as memory materials will be highlighted.

References and Notes

1. Examples include spin-crossover materials, transition metal oxides underdoing the metal-insulator transition, magnetic intermetallic alloys, manganites, charge density wave compounds, metal hydrides, ammonium chloride, quartz, transitions to incommensurate structures in dielectrics, and halide perovskites.
2. Tapas Bar, *et al.*, Phys. Rev. Lett. 121, 045701 (2018); S. Kundu, *et al.*, Phys. Rev. Lett. 124, 095703 (2020) ; S. Kundu, *et al.*, Phys. Rev. E 108, 024101 (2023).

IT-20

Quantum Coarsening Dynamics in Frustrated Magnetic Hamiltonians using Quantum Simulators

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Abstract: Geometric frustration in two-dimensional Ising models allows for a wealth of exotic universal behavior, both Ising and non-Ising, in the presence of quantum fluctuations. In particular, the triangular antiferromagnetic, Shastry-Sutherland and Villain model in a transverse field can be understood through distinct XY pseudospins, but have qualitatively similar phase diagrams including a quantum phase transition in the (2+1)-dimensional XY universality class. While the quantum dynamics of modestly-sized systems can be simulated classically using tensor-based methods, these methods become infeasible for larger lattices. Here we perform both classical and quantum simulations of these dynamics on triangular and villain modes, where our quantum simulator is a superconducting quantum annealer. Our observations on the triangular lattice suggest that the dominant quench dynamics obey a faster quantum coarsening dynamics in an effective two-dimensional XY model in the ordered phase. [1] Furthermore, we also showcase our recent results on Shastry Sutherland Lattice using a neutral atom platform. We perform these simulations in lattices which are larger than what is nominally possible by traditional methods to capture the dynamics at the quantum phase transition. These results demonstrate the ability of quantum annealers to simulate coherent quantum dynamics and scale beyond the reach of classical approaches. Most importantly the results help us test the results in new experiments using quenched fields on Ising quantum magnets using neutron scattering and magnetostriction experiments.

[1] A. Ali et al., https://doi.org/10.48550/arXiv.2403.00091, to appear in Nature Communication.

IT-21

Engineering collective quantum phenomena in oxide heterostructures

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Abstract: Interface engineering of complex oxides has become a popular approach to realize fascinating collective phenomena, which are very often "hidden" or unattainable in the constituent bulk materials. While the strong interplay among spin, charge, orbital, and lattice degrees of freedom facilitates interesting many-body quantum phenomena in correlated oxides, the additional broken symmetries and frustrated couplings across the interface of artificial heterostructures may give rise to new electronic, magnetic states. In this presentation, I will discuss our ongoing work on titanate, nickelate, and double perovskite-based heterostructure. The results of synchrotron diffraction, x-ray absorption spectroscopy, and hard X-ray photoemission spectroscopy to elucidate the response of underlying lattice, spin, orbital, and charge degrees of freedom due to heterostructuing will be presented.

IT-22

Tale of Iridates: How strong is the spin orbit coupling in reality

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Abstract: In spite of the relatively week in strength the role of the spin orbit coupling (SOC) turns out to be one of the most strategic energy scales in emerging novel quantum phases across the electronic, magnetic and topological phases of matter in various classes of quantum materials. Iridates are one such class of materials where both electronic correlation and spin-orbit interaction are competing, forms a new play ground for emerging field of research with huge promise for realizing different novel phases of matter such as quenched magnetic phases, spin-orbit Mott insulator, topological phases etc. It is common notion that for the iridates the SOC energy scales is the dominating factor in deriving Jeff states which eventually leads to the SOC enhanced Mott insulator over the conventional correlated Mott insulators. However, recently there are examples of iridates where the possibility of realization of Jeff state is not only determined by the SOC, rather competition with the other energy scales involved in the systems. This presentation is devoted to discuss few cases studies deals with the prediction and investigation of microscopic origin of emerged counter-intuitive challenging quantum phase due to the breakdown of strong spin-orbit coupling in the Iridium based transition metal oxides. These various novel phenomena arise due to interplay of charge, lattice, orbital and spin degrees of freedom, which are governed by the "electrons". Therefore, *ab-initio* electronic structure methodology have been used to understand such phenomena in general.

References

[1] K. C Kharkwal, R.Roy, H. Kumar, A. K Bera, S. M Yusuf, A. K Shukla, K. Kumar, S. Kanungo, and A. K Pramanik. Phys. Rev. B 102, 174401 (2020).
[2] Roumita Roy and S. Kanungo, Phys. Rev. B 106, 125113 (2022).
[3] S. Kanungo *et. al*.; Phys. Rev. B 93, 245148 (2016).
[4] S. Kanungo *et. al*. Angew. Chem. Int. Ed. 54, 5417 (2015)
[5] Roumita Roy and S. Kanungo, Phys. Rev. B 108, 155110 (2023)
[6] Roumita Roy and S. Kanungo, Phys. Rev. B 109, 085107 (2024)

IT-23

***In situ* Synchrotron Radiation Characterisation of the Incipient Growth of Functional Materials via Atomic/Molecular Layer Deposition**

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Abstract: Atomic layer deposition (ALD) and molecular layer deposition (MLD) are important and highly versatile growth techniques for a variety of thin film functional materials. ALD is unmatched in its ability to produce conformal films over large areas with thickness in the nanometre range[1]. A key consideration in many modern devices is the atomic structure of the heterointerface, which often ultimately governs the electronic or chemical process of interest. The structure of the deposit and its interface naturally depends on the atomic mechanisms that take place during growth, which for ALD have been difficult to study due to the near-atmospheric pressure. At the beamline SIRIUS of synchrotron SOLEIL, in partnership with collaborators from several French laboratories, we have developed a custom ALD/MLD reactor which mounts onto the heavy-duty diffractometer of the beamline[2]. In this presentation, we will show how the combination of *in situ* synchrotron radiation

characterisation (x-ray absorption, fluorescence, reflectivity, grazing incidence diffraction) and theoretical modelling is a powerful approach with unique potential for obtaining real-time structural and chemical information during the incipient ALD of a variety of functional and energy materials.
We will focus here on the study of the ALD of ZnO on several substrates and on the growth of transition metal dichalcogenides (TMD) using an original procedure mixing ALD and MLD. ZnO semiconductors have received attention because of desirable properties such as wide band gap energy, high exciton binding energy at room temperature, good conductivity and high transparency in the visible region; these features make ZnO thin films very suitable for room temperature ultraviolet optoelectronic devices application and as transparent conductive electrodes in solar cells[3]. TMD such as TiS_2 and MoS_2, lamellar materials with layers separated by van der Walls gaps which can be grown in form of ultra-thin "2D" films, are receiving great interest for potential applications in super-capacitors, batteries, electronics and optoelectronics[4]. For ZnO, we found that the growth behaviour, degree of local order, and crystalline texture depend strongly on the choice of substrate and on its different chemical preparation methods[2,5,6]. For TMD, we were able to understand the interactions of the precursor molecule with the substrate since the very first metal pulse of the ALD process and to prove the principle of the novel 2-step ALD/MLD synthesis, which separates growth and crystallization[7,8,9].
[1] M. Ritala *et al.*, *Science* 288, 319−321 (2000).
[2] R. Boichot *et al.*, *Chemistry of Materials* 28, 592–600 (2016).
[3] L. Schmidt-Mende and J. L. MacManus-Driscoll, *Materials Today* 10, 40−48 (2007).
[4] Y. P. Venkata Subbaiah *et al.*, *Adv. Funct. Mater.* 26, 2046−2069 (2016).
[5] M. H. Chu *et al.*, *Crystal Growth & Design* 16, 5339-5348 (2016).
[6] G. Ciatto *et al.*, *Crystal Growth & Design* 22, 4768–4776 (2022).
[7] P. Abi Younes *et al.*, *Chemistry of Materials* 34, 10885−10901 (2022).
[8] P. Abi Younes *et al.*, *Journal of Vacuum Science & Technology A* 41, 042403 (2023).
[9] A. K. Yadav *et al.*, *Nanoscale* 16, 1853-1864. (2024).

IT-24

In-Plane Anisotropy of Magnetic Textures Revealed by Planar Hall Effect

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The investigation of magnetic textures with non-coplanar ordering in bulk chiral magnets and thin-film heterostructures is a focal point in condensed matter physics due to the rich physical phenomena associated with topologically non-trivial states and low-energy excitations. Challenges arise in visually capturing the anisotropy of these textures, including the well-studied skyrmions. A prudent approach involves the examination of magnetotransport through the study of topological Hall effect. However, in our work, we utilized a less-explored planar Hall measurement configuration to examine the spin-canted state of a Heisenberg ferromagnetic insulator Europium sulfide (EuS) in $Bi_2(Se,Te)_3$/EuS bilayer devices. Our observation of planar Hall anisotropy, substantiated by theoretical investigations, thus far provides evidence for the existence of an unconventional magnetic phase in interfacial EuS, such as the elongated skyrmions, opening up promising new avenues in the development of next-generation topological spintronic devices.
References
1. Juhi Singh, Karthik V. Raman, and Narayan Mohanta, Phys. Rev. B 110, 125133, 2024
2. Dhavala Suri, Satyaki Sasmal, Archit Bhardwaj, Juhi Singh, Suman Mundlia, Anshika Mishra, Narayan Mohanta, and Karthik V. Raman, Phys. Rev. B 110, 134433, 2024

IT-25

Ferroelectric Films for Clean Energy Generation using Piezo and Tribo Effect

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Abstract: With the ever-increasing demand for energy and also due to an increase in environmental pollution, there has been a lot of interest in developing novel materials for clean energy generation. Ferroelectric materials have great potential for harvesting vibration energy through piezo/effects [1-2] which is a friendly approach to provide solutions to the present problem. The performance of piezo generator depends upon the properties of ferroelectric materials such as its dielectric constants and piezo-coefficient. We have simulated the performance of piezo generators and tested the output on PVDF-based nanocomposite ferroelectric films in which various parameters can be tuned [3]. It is also demonstrated that the performance of the piezo generator can also be enhanced by external perturbation such as magnetic field [4]. Tribo effect-based nanogenerators have also great potential for harvesting mechanical energy because of their robustness, cost-effectiveness, and higher performance. In the solid-solid interface-based tribo-nanogenerator both the material used for contact are solid [1] whereas in the solid-liquid interface-based tribo-nanogenerator liquid (water drop) comes in contact with a solid

material [5]. The performance of these tribo-nanogenerators depends upon the amount of induced charges during the contact and the retentivity of these charges which can be captured for generating electricity. We have designed nanocomposite and bilayer ferroelectric films which resulted in improving the generation of more surface charges and also capturing of the charges for longer time and thereby improving the performance of ferroelectric-based tribodevices [6]. Hybrid design of the devices which combines the piezo-tribo effect or tribo-thermoelectric effect is also demonstrated for getting higher output [1,7].
The present talk will review the progress made so far in our group at IIT Delhi in the above-mentioned area and will also present the main challenges.
Reference:
[1] H. H. Singh and N. Khare, Nano Energy, 52, 216-222 (2018)
[2] H. H. Singh, D. Kumar and N. Khare, Applied Physics Letters, 119, 053901 (2021)
[3] A. Mondal, M. Faraz and N. Khare, Journal of Electronic Materials, 53, 6933-6944 (2024)
[4] A. Mondal, M. Faraz, N. Khare, Applied Physics Letters, 121, 103901 (2022)
[5] H. H. Singh and N. Khare, Advanced Materials Interfaces, 8, 2170068 (2021)
[6] A. Mondal, M. Faraz, M. Dahiya and N. Khare, ACS Applied Materials & Interfaces, 16, 50659-50670 (2024)
[7] A. K. Gautam, HH Singh, N Khare, Nano Energy 107, 108125 (2023).

IT-26

X-ray-based investigations on interface engineered Neutron and X-ray multilayers

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Abstract: Interface property of neutron and X-ray thin film multilayers are very critical since both interface diffusion and interface roughness can degrade performance of a multilayer based device. An interface with sharp and high contrast of X-ray refractive index or neutron scattering length is desirable to reduce the scattering as well as increase the Fresnel's reflectivity to achieve high reflectivity. In our laboratory it has been demonstrated [1-7] that the reflectivities of neutron supermirrors and soft X-ray multilayer mirrors can be improved by interface engineering, either by introducing Air or N_2 gas along with Ar gas into the plasma during sputtering or by introducing a very thin barrier layer of C or B_4C at the interface of the two materials. To understand the physical and chemical properties of the engineered interfaces specular and diffused X-ray reflectivity using lab X-ray as well as grazing incidence EXAFS and grazing incidence XRF using Synchrotron X-ray are performed regularly. Along with these complementary techniques like cross sectional TEM and XPS are also done. In this presentation multilayer neutron mirrors deposited under only Ar ambience and $Ar+N_2$ ambience will be discussed. Studies have been carried out on as-deposited and annealed samples. Recrystallization of NiTi at the interfaces has been observed at higher annealing temperature and it has been found that the amorphous Ni/Ti multilayer is more preferable for recrystallization. This finding has been supported by molecular dynamics (MD) simulation of Ni/Ti multilayer. Along with this the effect of B_4C diffusion barrier on the interface of Cr/Sc [6] water-window soft X-ray multilayer and effect of C diffusion barrier on Mo/Si [4] EUV multilayer and W/Si [7] hard X-ray supermirror for X-ray space telescope application will also be discussed.

References

1. A. Biswas, Abharana N, S. N. Jha and D. Bhattacharyya, Applied Surface Science 542 (2021) 148733.
2. A. Biswas, Abharana N, S. Rai, and D. Bhattacharyya, J. Appl. Phys. 127 (2020) 165304.
3. Abharana. N, A. Biswas, P. Sarkar, S. Rai, S. Singh, S. Kumar, S.N. Jha, D. Bhattacharyya, Vacuum 169 (2019) 108864.
4. N. Abharana, A. Biswas, P. Sarkar, P. Rajput, De Rajnarayan, K. D. Rao, M. H. Modi, D. Bhattacharyya, S. N. Jha, N. K. Sahoo, Thin Solid Film, 673 (2019)126-135.
5. P. Sarkar, A. Biswas, N. Abharana, S. Rai, M. H. Modi and D. Bhattacharyya, J. Synchrotron Rad. 28 (2021) 224-230.
6. Piyali Sarkar, Arup Biswas, Ravi Kumar, Sanjay Rai, S Jha, Dibyendu Bhattacharyya, Physical Chemistry Chemical Physics 25 (2023) 3072.
7. Simran Atwal, P Sarkar, K Bhattcharyya, PN Rao, S Rai, Gurupada Ghorai, PK Sahoo, S K Ghosh, D Bhattacharyya, A Biswas, Applied Surface Science 657 (2024) 159736

IT-27

High Performance Thermoelectric Nanocomposites with 2D Graphene and MXene

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Abstract: Thermoelectric generators (TEGs) have emerged as promising technology for clean energy generation by directly converting waste heat into electrical power. However, it is challenging to design TEG with high energy conversion efficiency dictated by thermoelectric (TE) figure-of-merit, $ZT=S^2\sigma T/\kappa$ as it requires decoupling of electron and heat transport in solid bulk materials. One of the drawbacks of attaining better electron transport in polycrystalline bulk solids is the presence of 2-dimensional defects such as grain boundaries. Recently, we have shown that *ZT* values of thermoelectrics can be significantly enhanced by employing the strategy of making TE composites with highly conductive 2D materials such as graphene or MXene. We have used the matrix of various thermoelectric materials such as oxides, sulphides, skutterudites to make these composites. Challenges in oxide thermoelectrics are manifold as *ZT* values of oxides suffer from lower electrical conductivity as well as relatively higher thermal conductivity compared to intermetallics and chalcogenides. Electrons in oxide perovskites suffer from Anderson's localization due to the presence of multi-valent transition metals and point defects giving rise to variation in local electric field and strain. We have used the strategy of boosting the electron transport by manipulating semiconductor to metal transition temperature in donor doped $SrTiO_3$ by synthesizing nanocomposites with graphene, graphite and MXene. Presence of these inclusions in perovskite matrix provide high momentum electrons and impart enough strain to facilitate these localized electrons to attain the itinerant state. As a result, we could achieve single-crystal like electron mobility in ceramic nanocomposites. Furthermore, we could restrain the increase in thermal conductivity by attaining enhanced Umklapp scattering along with phonon-glass-like temperature-independent phonon mean-free-path above Debye temperature. We have fabricated 4-legged n-type thermoelectric power generator demonstrating milliwatt-level power output, hitherto remained unattainable for oxide thermoelectrics. Further we have synthesized composites of Bi_2S_3 and $CoSb_3$ Skutterudite with MXene and graphite to enhance their ZT values. The common observation from our study on incorporating highly conductive 2D materials in thermoelectric materials is the enhancement of electron transport by increasing carrier concentration and mobility. Most importantly the presence of these secondary phases in the composites induces enhanced phonon scattering, especially at high temperatures allowing us to achieve enhanced *ZT* values. Our proposed way of designing bulk composites with 2D materials can potentially open up the possibility of fabricating novel thermoelectric generators.

IT-28

Developing Safe, Cost Effective and High Energy Density Solid State Battery

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Abstract: With the popularity of next-generation high-end electronic devices and the promotion of electric vehicles (EV), the cutting-edge lithium-ion battery (LIB) technology has continuously run into one bottleneck or another. Its main performance metrics (including energy density, power density, cycle life, safety, cost, etc.) have been unable to meet the ever-tightening demands for electrified transportation as well as renewable integration into the electricity grid. For electric vehicles, the most important application field of LIBs, it is necessary to reach an energy density of at least 400 Wh/kg at scale. After more than 25 years of commercialization, especially after large-scale production and applications in recent years, many components of LIBs (such as current collector, separator, packaging, and the like) have remained unchanged. Therefore, the important performance metrics of LIBs are mainly determined by the electrode material and electrolyte. And more importantly, next-generation LIBs need reasonable matching of electrode and electrolyte to achieve the best performance, including longer cycling and better safety. I have identified these underlying causes for cost-effective, sustainable, safe, high energy density Li-ion battery.

- Next generation high energy and power density battery materials.
- Cost-effective cobalt-free Li-ion battery technology.
- Solid state (safe) battery technology.
- Advanced battery diagnostic tests and remanufacturing techniques.
- Advanced recycling systems that aim at expensive battery elements which include lithium, cobalt, nickel, manganese, etc.

These contributions are critical if energy storage technologies are to reach their full sustainability potential. Such studies will also enable Clean Technologies and Environmental Policy to continue its growth trajectory in impact

and global reach. I look forward to presenting the consequences solid-state battery technology on these contributions in my upcoming talk

Reference:

1. *Nature Energy volume 3, pages267–278(2018)*
2. *Nature Materials volume 19, pages1339–1345(2020*
3. *Chem. Rev. 2020, 120, 14, 6878–6933*
4. *Nature Nanotechnology volume 15, pages170–180(2020)*

IT-29

Interfacial Engineering for Advanced Wearable and Bulk Thermoelectric Devices

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Abstract: Sustainable Development Goal (SDG) 7 promoting equitable access to cheap, sustainable, and modern energy for everyone is directly aligned with the search for creative energy-harvesting solutions as the demand for clean and sustainable energy continues to rise globally. In order to accomplish these objectives, thermoelectric (TE) technologies which may directly transform heat into electricity or vice versa-offer a viable avenue[1]. This talk explores the bulk and wearable TE materials to transform energy efficiency and facilitates broad use in a variety of industrial domains. Wearable thermoelectric devices will power the portable gadgets, smart textiles, and health monitoring systems by capturing body heat, and rule the future generation through internet of things (IOT)[2,3]. The advancements of in-situ grown nanostructured materials and organic-inorganic hybrids are examined, with a focus on their potential for incorporation into scalability[2]. Especially, the interface plays the major role on energy filtering effect and polarization effect to enhance the conversion efficiency. However, bulk thermoelectric systems show a great deal for recovering waste heat in the automotive and industrial sectors. The interdependent properties of charge carrier and phonon dynamics are significantly affecting the TE performance. The following strategies will be used to regulating the properties of TE materials, i) altering of band structure through doping, ii) confining the band valley degeneracy by alloying, and iii) regulating the phonon propagation by organic-inorganic hybrid composites, and nano structuring respectively[4–6].

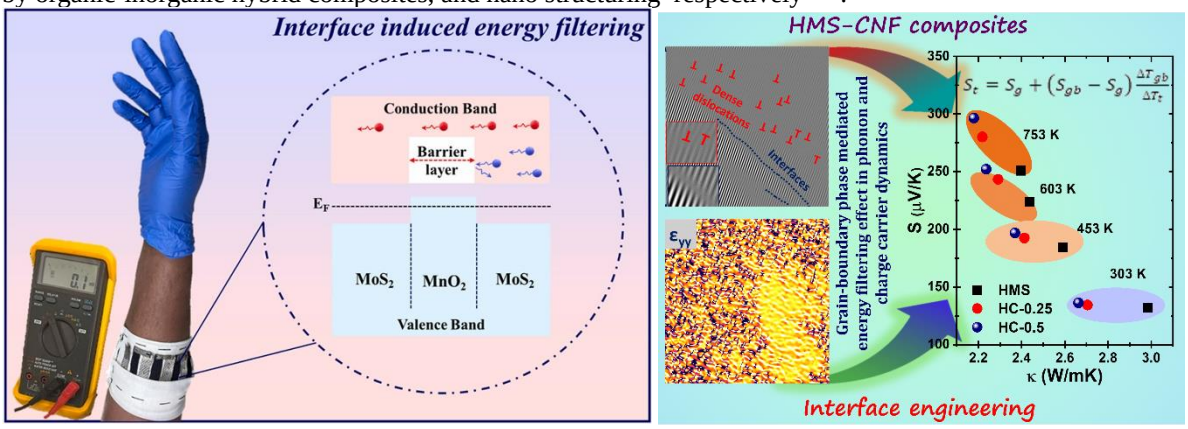

Figure: Interfacial energy filtering effect in wearable (1D-2D compounds) and bulk (grain-boundary phase) thermoelectric materials.

References:

[1] X. L. Shi, J. Zou, Z. G. Chen, *Chem. Rev.* **2020**, *120*, 7399.

[2] C. Suresh Prasanna, S. Harish, J. Archana, E. Senthil Kumar, H. Ikeda, M. Navaneethan, *Carbon N. Y.* **2024**, *218*, 118609.

[3] J. Vinodhini, S. Harish, H. Ikeda, M. Navaneethan, *Surfaces and Interfaces* **2024**, *54*.

[4] S. Priyadharshini, V. Vijay, S. Kamalakannan, J. Archana, M. Navaneethan, *Appl. Phys. Lett.* **2024**, *124*, 031601.

[5] M. J. K. P., S. S. John, A. J., H. S., N. M., *Appl. Phys. Lett.* **2024**, *125*, 34101.

[6] V. Vijay, J. Karuna, J. Archana, M. Navaneethan, *Appl. Phys. Lett.* **2024**, *125*, 171603.

IT-30

Ultrafast terahertz dynamics in solids and interfaces

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Abstract: Femtosecond laser pulses can be used to induce and simultaneously study nonequilibrium dynamics of different types of coherent excitations in solids. The coherent dynamics of the excitations of charge entities can construct real physical currents that they mimic sources of a new electromagnetic radiation whose frequency is determined by the time scale involved in the coherent dynamics of the excitations. Our group is interested in learning about light matter interaction at ultrafast time scales through THz pulse generation from solids and use it as a probing tool for investigating various intrinsic dynamical processes going on during and after the light matter interaction in technologically relevant material systems. In this talk, I will discuss a few results [1-3] on thin metallic film heterostructures and three-dimensional topological insulators and try to convey some of the above connections.

[1] Sandeep Kumar and Sunil Kumar, iScience 25, 104718 (2022).
[2] Sandeep Kumar and Sunil Kumar, Nature Communications 14, 8185 (2023).
[3] Anand Nivedan and Sunil Kumar, New Journal of Physics 26, 033044 (2024).

IT-31

Topological Semimetals Under Intense Laser: A Route to Anisotropic Nonlinear Hall Effect

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Discoveries of topological materials, such as topological insulators, Dirac, and Weyl semimetals, have revolutionized contemporary physics. Moreover, these materials offer exciting opportunities for upcoming quantum technologies and opto-electronics. In this talk, I will show how intense laser-driven electron dynamics in topological Weyl semimetals have many intriguing features. The first interesting observation will be discussed that the parity and magnitude of the non-trivial Berry curvature's components control the direction and strength of the anomalous current, which leads to the generation of anomalous odd-order harmonics [1,2]. In the later part, I will emphasize the generation and tailoring of photocurrent in Weyl semimetals. It is well-known that circularly polarized light fails to generate photocurrent in inversion-symmetric Weyl semimetals with degenerate Weyl nodes. While each node generates a current with a direction depending on its chirality, the two currents in the two degenerate nodes of opposite chirality cancel each other. By extension, it is also generally expected that the currents generated at the same Weyl node by the fields of opposite helicity should also observe mirror symmetry and cancel. Surprisingly, this is not the case. The origin of this effect lies in the nonlinear energy dispersion, which manifests strongly already remarkably close to the Weyl nodes, where linear dispersion is expected to hold, and the Weyl fermions are thus expected to be massless [3]. As an application of this phenomenon, we introduce a method to generate helicity-sensitive photocurrent in Weyl semimetals with degenerate Weyl nodes at the Fermi level [3-5].

References:

[1] A. Bharti, M. S. Mrudul and G. Dixit, Phys. Rev. B 105, 155140 (2022).
[2] A. Bharti and G. Dixit, Phys. Rev. B 107, 224308 (2023).
[3] A. Bharti, M. Ivanov and G. Dixit, Phys. Rev. B 108, L020305 (2023).
[4] A. Bharti and G. Dixit, Phys. Rev. B 108, L161113 (2023).
[5] A. Bharti and G. Dixit, Phys. Rev. B 109, 104309 (2024).

IT-32

Pressure-induced structural modifications in Remeika phase quasi skutterudite stannides

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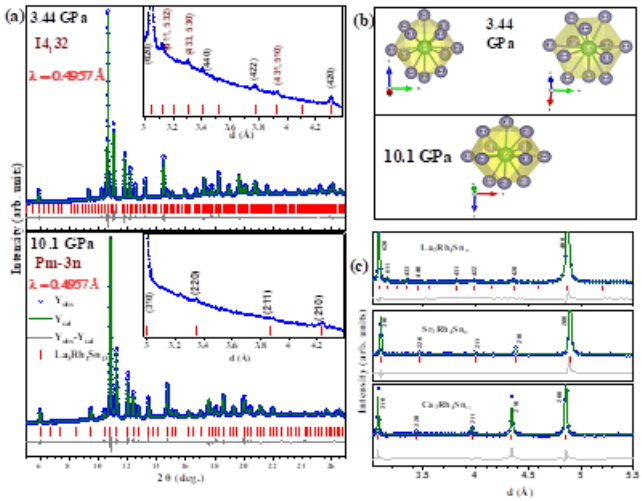
Abstract: The intermetallic stannides with formula $R_3T_4Sn_{13}$ (3-4-13) and $R_5T_6Sn_{18}$ (5-6-18) (where R= rare-earth/alkali metal; T = transition-metal) are attracting much attention due to their peculiar cage-like structure as well as interesting physical properties, particularly superconductivity. Recently we are involved in the high-pressure Raman and structural studies of several of these systems [1-4]. These studies are conducted at the Indo-Italian beamline Xpress at the Elettra synchrotron radiation facility. Present status of this facility will be presented. The status of the on-going synchrotron upgrade program at Elettra will also be touched upon.

Figure 1: (a): Results of the Rietveld refinement analysis of the x-ray powder diffraction patterns of $La_3Rh_4Sn_{13}$ at 3.44 and 10.1 GPa. The inset shows a zoom over selected *d*-spacing, allowing for a clear view of superlattice peak suppression in the HP phase. (b) The local structure around La at high and the low-pressure phases. (c) A

zoom over the diffraction pattern for $La_3Rh_4Sn_{13}$, $Sr_3Rh_4Sn_{13}$ and $Ca_3Rh_4Sn_{13}$ together with the Rietveld refinement results (with x-axis in d-spacing (Å)) at ambient conditions. Here, $Sr_3Rh_4Sn_{13}$ and $Ca_3Rh_4Sn_{13}$ have identical Bragg reflections, whereas $La_3Rh_4Sn_{13}$ presents several additional weak reflections in-agreement with the lattice doubling.



References
[1] Lingannan G, et al., *J. Phys.: Condens. Matter* (2022); **34** 245601
[2] Sundaramoorthy M, et al., *Phys. Status Solidi RRL* (2023); **17** 2300078
[3] Sundaramoorthy M, et al., *J. Alloys Compounds* (2024); **973** 172905
[4] Sundaramoorthy M, et al., *Chem. Phys. Chem.* (2024); **25** e20240286

IT-33

Correlation between magnetic structure and magnetoelectric properties of the green phases R_2BaCuO_5 (R=Rare-earth)

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The origin spin-induced multiferroicity is typically the magnetic symmetry within transition metal ions. However, ordering rare-earth elements also plays a critical role in inducing electric polarization, mediated by exchange interactions between rare-earth and transition metal ions. In this presentation, I will discuss the magnetic and magnetoelectric properties of the green phases R_2BaCuO_5. In these materials, interactions between rare-earth ions and Cu govern the magnetic structure, resulting in diverse magnetoelectric behaviors. For instance, the k=0 magnetic structure in Sm_5BaCuO_5 induces a linear magnetoelectric effect, while Gd_2BaCuO_5 exhibits spontaneous electric polarization through cycloidal ordering, followed by a polar commensurate ground-state magnetic structure. Compounds such as Dy_2BaCuO_5 and Ho_2BaCuO_5 demonstrate a linear magnetoelectric effect below their magnetic ordering temperatures, which extends to metamagnetic transitions. Above these temperatures, both compounds show pronounced magnetization and electric polarization. I will also present the opportunities to perform neutron and muon experiments at the ISIS facility of the Rutherford Appleton Laboratory, UK, as part of the DST-STFC collaboration.

1) P. Yanda, N. V. Ter-Oganessian and A. Sundaresan, Linear Magnetoelectric Effect in Antiferromagnetic Sm2BaCuO5, Phys. Rev. B, 100, 104417 - 104420 (2019).
2) P. Yanda, I. V. Golosovsky, I. Mirebeau, N. V. Ter-Oganessian, Juan Rodríguez-Carvajal, and A. Sundaresan, Interplay of 4f-3d interactions and spin-induced ferroelectricity in the green phase Gd2BaCuO5, Phys. Rev. Research 2. 023271 (2020).
3) P. Yanda, F. Orlandi, P. Manuel, N. Boudjada, Juan-Rodrigue Carvajal, and A. Sundaresan, Magnetic field induced ferroelectric state in centrosymmetric R2BaCuO5 (R=Dy and Ho) Phys. Rev. B (2021).
4) Swarnamayee Mishra, P Yanda, Shrikant Bhat, Martin Etter, and A. Sundaresan, Highpressure synthesis, and magnetic properties of tetragonal R2BaCuO5 (R= Sm and Eu) Frontiers in Chemistry 11, 116645 (2023).

IT-34

Entangled orbital, spin and ferroelectric order in cesium superoxide

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Abstract: CsO_2 belongs to the family of alkali superoxides (AO_2, where A = Na, K, Rb, and Cs). These compounds exhibit magnetic behaviour due to open p-shell electrons on O_2- molecules [1], resulting in an effective s=1/2. Because these molecules have finite size and an orientational degree of freedom, there is strong coupling between the crystal structure and the magnetism, and good reason to believe that the magnetic interactions are highly anisotropic.
Using neutron diffraction [2], we elucidated the crystal and magnetic structures of CsO_2. Our observations reveal a complex series of structural changes as temperature decreases from room temperature to 1.6 K. These include an incommensurate modulation in the crystal structure, followed by a lock-in transition that doubles the unit cell compared to the previously assumed orthorhombic unit cell [3]. In both cases, our structural analysis indicates a staggering of caesium ion positions along the b-axis, distinct from other alkali superoxides where staggered tilts of the O_2- dimers are observed. Below 10 K, we detected magnetic Bragg peaks and refined an antiferromagnetic structure with magnetic moments predominantly aligned along the b-axis, with a minor component along the a-axis that strongly implies anisotropic exchange coupling.
Inelastic neutron scattering measurements reveal a rich magnetic excitation spectrum that can be explained by a strong exchange coupling along two of the eight body diagonals of the parent tetragonal structure. This means that CsO_2 can be regarded as a staggered 1-dimensional spin-1/2 chain, although the chain axis is perpendicular to that assumed in analysis of previous NMR [3] and bulk susceptibility measurements [2]. Our results are supported by recent theoretical work that uses a combination of ab-initio Hubbard models and superexchange theory. Here, orbital order gives rise to the observed anisotropic exchange coupling, as well as the possibility of magnetically induced ferroelectric polarisation.
These results point to CsO_2 being an interesting example of a structure-properties relationship, and may indicate a new avenue for engineering the anisotropic exchange needed for effects such as multiferroicity or Kitaev spin liquid physics.
[1] W. Hesse et al, Recent results in solid state chemistry of ionic ozonides, hyperoxdies and peroxides, Prog. Solid State Chem. ***19****, 47 (1989)*
[2] Crystal and magnetic structure of cesium superoxide, R. A. Ewings et al, Phys. Rev. B ***108****, 174412 (2023)*
[3] Antiferromagnetic S=1/2 spin chain driven by p-orbital ordering in CsO_2, S. Riyadi et al, Phys. Rev. Lett. ***108****, 217206 (2012)*
[4] Phonon-modulated magnetic interactions and spin Tomonaga-Luttinger liquid in the p-orbital antiferromagnet CsO_2, M. Klanšek et al, Phys. Rev. Lett. ***115****, 057205 (2015)*

IT-35

Neutron diffraction: An unambiguous tool for characterizing magnetism in emerging materials

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Abstract: Advanced material sciences research involves designing and investigating novel materials with exotic magnetic property towards their potential technological application and further understanding intriguing physics behind exotic properties. Beside this, interpreting Quantum behavior in materials is another fascinating aspect in matter with can exhibit fractionalized excitations and drawing attention of research community. Several materials are being vigorously explored for realizing quantum state and their potential applications in quantum computers [1-3]. The exact knowledge to ground state assumes significant in such compounds. The neutron diffraction is a unique technique to study crystal, magnetic structure and locating neighboring constituent element more precisely. This information can be integrated with other physical properties in ensuring detailed correlation with structure of compound for explaining phenomenon extensively, thus providing valuable input in understanding ground state.
In this talk, importance of neutron diffraction as characterizing tool for magnetism will be discussed along with focussing crystal diffractometer (PD-3) beam line, installed by UGC-DAE CSR Mumbai Centre at Dhruva, BARC. Further, some recent results on emerging material such as heusler, 2 D kagome and few other interesting compounds will be discussed [4-9], highlighting importance of diffraction experiments in understanding physical properties more comprehensively.
References:
1. M. B. Sanders, J. W. Krizan and R. J. Cava, J. Mater. Chem. C, 4, 541 (2016)
2. Z. L. Dun, J. Trinh, M. Lee,E. S. Choi, K. Li, Y. F. Hu, Y. X. Wang, N. Blanc, A. P. Ramirez, and H. D. Zhou, Phys Rev B 95, 104439 (2017)
3. Z.-F. Ding, Y.-X. Yang, J. Zhang, C. Tan, Z.-H.Zhu, G. Chen and L. Shu, Phys Rev B 98, 174404 (2018).
4. S. Gupta, S. D. Kaushik et. al. Jour of Magn. Magn. Mater. 583 (2023) 170992
5. R. Harikrishnan, S. D. Kaushik et. al. Phys. Rev. B 108 (2023) 094407

6. R.A. Saha, S. D. Kaushik et. al. Phys. Rev. B 107 (2023) 155105
7. N. Kumar, S. D. Kaushik et. al. Crystals 13 (2023) 503
8. P. Aich, S. D. Kaushik et. al. Chem Mater. 35 (2023) 991
9. A. Shaw, S. D. Kaushik et. al. Jour of Magn. Magn. Mater. 488 (2019) 165338.

IT-36

Field Tunable band topology and topological Hall effect in skyrmion crystals

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Abstract: The topological Hall conductivity (THC) arises out of spin-asymmetric deflection of charge carriers flowing through a non-collinear spin system. Here, we show that band topology and THC in a skyrmion crystal can be tuned by changing the strength of the applied field driven Rashba spin-orbit coupling (RSOC). This results in the change of the subband Chern numbers and a transition between ordinary and Chern insulators. For partially filled subbands, the RSOC can tune the THC and reverse its sign so that the direction of the Hall current is flipped. The critical RSOC for this depends on the skyrmion type and the carrier density. We extend our analysis to the cases of Dresselhaus and Weyl SOC as well and show that they can be directly mapped to the RSOC case, which will, therefore, lead to similar results. The tunable charge transport in skyrmion crystals provides new promising avenues for spintronic applications.

References:

1. A. Mandal, S. Satpathy, and B. R. K. Nanda, arXiv: 2411.06434
2. P. Sahu, B. R. K. Nanda, and S. Satpathy, Phys. Rev. B, 106, 224403 (2022).

IT-37

Hidden Berry curvature and planar Hall effect in 2D materials

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Abstract: The planar Hall effect in 3D systems is an effective probe for their Berry curvature, topology, and electronic properties. However, the Berry curvature-induced conventional planar Hall effect is forbidden in 2D systems as the out-of-plane Berry curvature cannot couple to the band velocity of the electrons moving in the 2D plane. Here, we demonstrate a unique 2D planar Hall effect (2DPHE) originating from the hidden planar components of the Berry curvature and orbital magnetic moment in quasi-2D materials. We identify all planar band geometric contributions to 2DPHE and classify their crystalline symmetry restrictions. Using gated bilayer graphene as an example, we show that in addition to capturing the hidden band geometric effects, 2DPHE is also sensitive to the Lifshitz transitions. Our work motivates further exploration of hidden planar band geometry-induced 2DPHE and related transport phenomena for innovative applications.

IT-38

Polymer nanocomposite membranes for gas separation and sensing

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Abstract: In the dynamic landscape of industrial processes, membrane technology offers a paradigm shift beyond energy-intensive separation techniques, exemplifying a progressive leap toward sustainability. Hydrogen separation is critical for applications spanning clean energy production to gas purification. Membrane technology emerges as a cost-effective and efficient solution for achieving this goal. Enhancing membrane performance through the development of gas-sensitive materials is a key focus. Functionalization improved the membranes' surface properties and adhesion capabilities, enabling better integration of nanoparticles. It will help to improve the permeability and selectivity of membrane for the target gas. We also explored an eco-friendly and one-step route for the chemical synthesis of hierarchical polypyrrole (PPy) nanotubes assembled urchins and flower-like nanostructures via a template-assisted method and examine their morphology-dependent gas sensing characteristics. The ammonia sensor was mounted on low-cost and highly flexible polyvinylidene fluoride (PVDF) membrane substrate for the fabrication of flexible sensor. The proposed flexible gas sensor remarkable performance to detect ammonia at room temperature indicates its tremendous potential for wearable electronics applications.

Keywords: Membrane, Gas sensor, Flexible sensors

CONTRIBUTORY PAPERS

a) PHASE TRANSITIONS AND DYNAMICS

a0001

The Emergence of Density Wave and Supersolid Phases in Driven Optical Lattice

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In a periodically shaken lattice, bosons are transferred from the ground state to the excited band when the shaking frequency is increased. Motivated by the idea that the excited atom may be treated as a Rydberg atom, we study the two-band extended Bose Hubbard model by considering the nearest-neighbor interactions for the excited band boson using the CMFT+DMRG method. In our calculations, we obtain the superfluid order parameter and the boson density for the lower band and the excited band and identify the underlying Mott insulator (MI), π-superfluid ($\pi - SF$), the Density Wave (DW), and the Supersolid (SS) phases. The DW phase and the SS phase are due to the nearest neighbor interaction and the intra-band interactions. Density of bosons play very important role in the determination of the DW and the SS phases.

a0003

Neutron Diffraction Studies of (Ba, Ca)TiO_3 modified $NaNbO_3$ at Elevated Temperature

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Sodium niobate, a promising material for energy storage, has been transformed into a room-temperature ferroelectric phase through a well-known crystal engineering technique. This involved strategically substituting atoms within the crystal structure (A and B sites) to induce chemical pressure. The resulting material exhibits enhanced polarization strength at elevated temperatures, with the underlying mechanism linked to atomic displacements and octahedral rotation or distortions within the crystal lattice. This connection between structure and properties is further supported by the good agreement between computed polarization values and experimental data. Interestingly, the research also unveils the material's temperature-dependent phase transitions, transitioning from a ferroelectric phase at room temperature (***P****mc2*$_1$) to a high-symmetry paraelectric phase (***P****m-3m*) as temperatures increase. This work opens exciting possibilities for developing novel energy storage devices utilizing this engineered ferroelectric material.

a0004

Structural Phase Transition in Yttrium: Comparison of Exchange-correlation Functionals

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The structures of yttrium metal up to 30 GPa have been revisited using first-principles calculations. Focusing on the correct energetics and vibration frequencies we compared results of generalized gradient approximation (GGA), meta-GGA functionals. For GGA, Perdew-Burke-Ernzerhof (PBE) and for meta-GGA, strongly constrained and appropriately normed (SCAN) and r^{2}SCAN functional were considered. The PBE-GGA highly underestimates the structural phase transition pressure. The r^{2}SCAN functional provides accurate result for low pressure transition and underestimate the high-pressure transition. Going beyond static level, the vibration frequency of Y calculated by r^{2}SCAN functional is matches well with the experimental results. Our results emphasise that the introduction of soft modes in phonon dispersion curves might be the reason behind the structural phase transition in Y and significantly contribute to the area of high pressure by theoretical prediction of more accurate transition pressure.

a0005

Structural Stability of $GdTe_{1.75}$ Under Pressure

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The structural stability and compressibility behaviour of $GdTe_{1.75}$ was investigated using diamond anvil cell up to 25 GPa by high pressure x-ray diffraction experiments. $GdTe_{1.75}$ is synthesized in single phase by isopiestic vapour pressure technique. At ambient, $GdTe_{1.75}$ crystallizes in a tetragonal (P4/*nmm*) phase. The sample does not exhibit any structural transition up to the maximum pressure studied. The P-V data exhibits an anomalous compressibility

behavior. $GdTe_{1.75}$ is found to have different bulk moduli of 53 ± 3 GPa and 31 ± 5 GPa below and above the pressure of ~ 10 GPa. This is associated with similar anomalous behavior in *c*-axis variation with pressure.

a0006

Near Zero and Negative Linear Compressibility in Hybrid Organic-Inorganic Perovskite

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Hybrid organic-inorganic perovskites $[NH_2NH_3][Co(HCOO)_3]$ have a so-called "wine-rack" type of geometry that could give origin to the rare property of near zero and negative linear compressibility, which is an exotic and highly desirable material response. We use first-principles density functional theory computations to probe the response of these materials to hydrostatic pressure and predict near zero linear compressibility of 0.6 TPa^{-1} in 0-1 GPa range and negative linear compressibility of -2.7 TPa^{-1} in 1-6 GPa pressure range. Calculations reveal that, under pressure, CoO_6 octahedra and -HCOO ligands remain relatively rigid while CoO_6 octahedra tilt significantly, which leads to highly anisotropic mechanical properties and expansion along certain directions.

a0007

Investigation of Phonon Across Magnetic Phase Transition in Multiferroic $LuFeO_3$

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We report detailed temperature-dependent inelastic neutron scattering and ab initio lattice dynamics investigation of magnetic perovskites LuFeO3. Ab initio lattice dynamics calculations performed with different magnetic interactions show that the effect on specific phonon modes. The pressure-dependent DFT calculations are used to investigate the high spin to low-spin transition in LuFeO3, which is in excellent agreement with the available experimental data.

a0008

Topological Phases Of Non-Linear 1D Kitaev Chain Using Quench Dynamics

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The p-wave Kitaev chain in one-dimension hosts unpaired Majorana fermions in the topological phase. We employ quench dynamics to detect the topological phase using non-linearity induced time dependent differential equations of Majorana state wavefunctions, governed by the Hamiltonian involving Majorana pairing. Two different phase diagrams corresponding to the trivial and topological phase have been obtained using the time evolution of the Majorana states in the weak non-linear region.

a0009

Effect of TeO_2/SeO_2/Al_2O_3 on Thermal and Structural aspects of LGS Glass-ceramics

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The $25Li_2O$-$10GeO_2$-$60SiO_2$-5R (R= TeO_2, SeO_2, Al_2O_3) were synthesized by melt-quenching method. X-ray diffraction (XRD) analysis confirmed the ceramic nature of the synthesized samples. Energy-dispersive X-ray spectroscopy (EDS) was employed to determine the elemental composition of the samples. From the Matusita model corresponding to Differential Thermal Analysis (DTA), it was found that the activation energy of crystallization (E_c) is 285.49 kJ/mol at 10°C/min. The Avrami index (n) is 2 for the 5 mol% Al_2O_3 doped sample, indicating a slight predominance of bulk crystallization over surface crystallization. The sample was doped with 5 mol% of Al_2O_3 and had superior thermal stability.

a0011

Investigation Of Magnetocaloric Effect In A New Perovskite Oxide $La_{0.8}Ca_{0.2}Mn_{1-x}Co_xO_3$ (For x = 0 And 0.1)

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The prospect of $La_{0.8}Ca_{0.2}Mn_{1-x}Co_xO_3$ (for x = 0 and 0.1) perovskite oxides as magnetocaloric effect (MCE) based magnetic refrigerant has been investigated in terms of entropy and specific heat measurement. A phenomenological model has been adopted for the investigations of different magnetocaloric properties like magnetic entropy change, heat capacity change through the study of temperature dependence of magnetization. The results indicate the compounds as potential candidates for cooling system in a wide temperature interval in the vicinity of room temperature. Moreover, the results confirm the extent of validity of the phenomenological model.

a0013
Structural and Raman Studies on Ca_2MnTiO_6
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Double-perovskite oxide compound Ca_2MnTiO_6 (CMTO) have been synthesized using two-step solid state reaction method, i.e., by mixing two single perovskite phases $CaMnO_3$ (CMO) and $CaTiO_3$ (CTO) to understand correlation between structure and physical properties. A comparative study using Raman spectroscopy has been undertaken to understand the structural features of $CaMnO_3$, $CaTiO_3$ and Ca_2MnTiO_6 compounds at the microscopic level.

a0014
Orbital Magnetic Field Driven Phases in the Spin-1/2 Falicov-Kimball Model on A Triangular Lattice
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Numerical and Monte-Carlo simulation methods are employed to study the spin-1/2 Falicov-Kimball model on triangular lattice in the presence of external magnetic field. It is found that a metal to insulator transition accompanied by segregated phase to regular/mixed phase takes place with change in the magnetic field at small values of onsite Coulomb correlation. At large values of Coulomb correlation no metal to insulator transition is observed with variation of magnetic field. Electric and magnetic sensors and high energy storage devices can be developed using these results.

a0017
Symmetry Reentrant Phase Transition in Ag_4SSe at High Pressure
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Chalcogenides are technological important materials having several intriguing physical phenomena along with possibility of novel electronic and spintronic states. Ag_4SSe is one such material in this system. Angle dispersive x-ray diffraction studies have been performed on this material up to ~35 GPa during compression and decompression using x-rays from synchrotron source. It undergoes to a structural phase transition at 3.4 GPa (started at 1.5 GPa) pressure to a new high pressure orthorhombic phase which is determined to be in space group $P2_12_12_1$. Thus, the new high pressure phase shows a symmetry ascent kind of transformation which is generally unusual in high pressure studies. The nature of this structural phase transition is determined to be of first order. At further high pressures beyond 9.3 GPa it undergoes another phase transition to a new phase. This transition is completed by ~ 16.6 GPa. The second high pressure phase consists of crystalline planes with larger d spacing which implies the possibility of larger unit cell, possibly with the cell doubling mechanism for the second high pressure phase. Thus, Ag_4SSe shows symmetry ascent to symmetry decent type of transition on compression reflecting the symmetry re-entrant type of phase transition in this material.

a0018
Semiconductor-Metal like transition in Mg_2Si at High Pressure
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Study of energy efficient and technologically advanced materials is need of the our due to rising energy demand of the world. Alkaline earth silicides are significantly important thermoelectric materials which can generate electricity from waste heat from various processes. Mg_2Si is one such material of importance. Here, in this manuscript, magnesium silicide (Mg_2Si) has been investigated by in-situ Raman scattering measurements at high pressure. The detailed data analysis shows that it undergoes a phase transitions at ~ 7.1 GPa to a new high pressure phase HPI. Interestingly at highest pressure i.e. at 14.3 GPa, all the modes disappear except a very weak Raman mode at ~ 580 cm-1. This could be a possible signature of metallization of Mg_2Si in the high pressure phase. On release of pressure the Raman modes reappear implying the reversibility of this phase transition.

a0019

High Pressure Structural Investigation on Layered Metallic Delafossite $PdCoO_2$

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In this study, we report the effects of pressure on the structural properties of a layered metallic delafossite $PdCoO_2$ using synchrotron based powder X-ray diffraction (XRD). The XRD analysis reveal the stability of the ambient trigonal phase ($R\bar{3}m$) at least up to ~ 24 GPa. However, it exhibits anisotropic compression, with a-axis being the more compressible direction. This anisotropic compression increases with pressure, suggesting the mechanical stability of the octahedral sandwich layers and O-Pd-O dumbbell bonds. Nevertheless, anomalies in crystal anisotropy and inter-layer and intra- layer separation between octahedral planes indicate an isostructural transition at ~ 6.5 GPa. The pressure vs. volume data was fitted with 3rd order BM-eos and the obtained bulk modulus and its pressure derivative at ambient pressure are B_0= 235.9 (12) GPa, and B_0'=4.3 (1), respectively.

a0020

Harnessing Non-Stoichiometry in Pyrochlore to Tailor Structural and Thermophysical Properties

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To explore the significant impact of non-stoichiometry while avoiding heterovalent substitution, on the structural and thermophysical properties of pyrochlore materials, a series of Zr-rich, non-stoichiometric $Nd_{2-x}Zr_{2+x}O_{7+x/2}$ (x = 0, 0.2, 0.4, 1.2) pyrochlores was synthesized through hybrid gel combustion method. X-ray diffraction analysis revealed that compositions with x = 0, 0.2, and 0.4 exhibit a pyrochlore structure, while x = 1.2 displays a defect fluorite structure. Raman spectroscopy uncovered the presence of local disordered fluorite-type domains within the ordered pyrochlore matrix, creating a hybrid structure that reduces thermal conductivity. This study highlights the strategic manipulation of non-stoichiometry to tailor thermophysical properties without addition of any hetero-dopant, paving the way for the development of advanced thermal barrier materials with superior properties.

a0022

Phase transition in Zr and Nb substituted Zr under pressure: *Ab-initio* study

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Understanding the effect of Nb addition on the structural, mechanical and thermodynamic properties of Zr claddings is critical for nuclear reactor service safety. In the present work, we have investigated the phase diagram of Zr up to 40 GPa as well as Nb as substituted Zr using the first-principle electronic band structure method. In pure Zr, our calculation predicts alpha (α) to omega (ω) and omega (ω) to beta (β) transitions at pressures of 0.5 GPa and 27.5 GPa respectively. With inclusion of temperature (at 300 K) α to ω the transition pressure occurs at 1.2 GPa, which agrees with experimental value of ~2 GPa. In case of Zr-2.77%Nb our calculation predicts ω phase to be a stable at 0 K but at higher temperature of 600 K, α phase became stable over ω phase, similarly omega to beta transformation takes place at pressure 22.5 GPa. Our lattice dynamical calculations produce experimental phonon dispersion curve for α phase in Pure Zr, β-Nb and also predicts the dynamical stabilization of Zr-2.77%Nb at ambient condition which support our static lattice calculations.

a0023

On Response of Polycrystalline Copper under Dynamic Loading

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Plate impact experiments have been carried out in electrolytic-tough-pitch (ETP) 0.9995 polycrystalline copper (Cu) using 60 mm bore Gas Gun facility to measure various strength properties such as the Hugoniot Elastic Limit (HEL), dynamic yield strength and spall strength under shock loading conditions. The variation of the strength properties with dynamic stresses ranging from 3.5 to 14.4 GPa has been determined using interferometric techniques. The yield strength has been found to vary from 0.184-0.367 GPa in this pressure range as compared to quasi static value of 68 MPa (~3-5 times increase under shock loading of copper sample). The spall strength lies between 0.9 to 1.2 GPa in the same peak dynamic stresses range (with almost 3-4 times increase as compared to static tensile strength of 300 MPa).

a0024

High Temperature Vibrational and Photoluminescence Study of $SmNbO_4$

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Rare earth orthoniobates are well-known for their interesting structural, electrical, and optical properties, which make them valuable for various technological applications. Among them, $SmNbO_4$ has been studied for its optical and electrical properties. Despite its technological significance, its behavior under non-ambient conditions has not been extensively investigated. This study aims to explore the vibrational and photoluminescence (PL) properties of $SmNbO_4$ to gain insights into its phonon and electronic behavior at elevated temperatures. Raman spectroscopy reveals a discontinuous shift in the rate of change of mode frequencies at approximately 200°C and 520°C. The shift observed at ~200°C may be due to the changes in local lattice structure, while the discontinuity at ~520°C is indicative of a phase transition, as evidenced by the emergence of a new mode at this temperature. PL studies show a broadening of emission peaks, suggesting increased phonon-mediated recombination. These findings provide valuable insights into the phase transition in $SmNbO_4$ and its impact on the material's vibrational and optical properties.

a0026

Investigation of Structural Phase Transition in α-In_2Se_3 Using Raman Spectroscopy

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Chalcogenide materials have received a considerable attention for their exceptional physical, electrical, and optical properties, which made them ideal candidate for next-generation optoelectronic devices. Raman spectroscopy is an advanced technique for characterizing materials and comprehending microscopic changes, such as soft chemical bonds associated with vibrational modes and electronic transitions. In this regard, In_2Se_3, is a well-known layered material, which has a considerable polymorphic structure that can change with external parameters such as temperature, pressure, and magnetic field. Such external stimulations make it an ideal material to understand the phonon dynamics. In this work, we have obtained thin layer of In_2Se_3 using mechanical exfoliation and emphasized on the structural phase transition through temperature dependent Raman spectroscopy.

a0027

Effect of Sm^{3+}on the Structural, Dielectric And Thermal Stability In Bi-layered Structure $SrBi_4Ti_4O_{15}$ Ceramics

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$SrBi_{4-x}Sm_xTi_4O_{15}$ (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.

a0028

Topological Phase Transition in two-leg SSH ladder with Further Neighbor Hopping

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This study explores the phase transition in a two-leg-coupled Su-Schrieffer-Heeger (SSH) chain incorporating extended next-nearest-neighbor (NNN) terms. We have already seen the effects of intra-cellular and inter-cellular hopping terms, denoted as v and w, respectively, alongside the coupling terms t_1 *and* t_2 that link the two one-dimensional SSH chains. We will investigate the influence of additional NNN terms t_3 *and* t_4 within each leg of the chain. Previous research has shown that without these extended terms, the winding numbers (W) of the system ranges from -1 to 1. Our analysis reveals that by varying the coupling parameters, the winding numbers (W) can shift from -2 to +2, uncovering new topological phases. Furthermore, introducing extended NNN terms causes the winding numbers (W) to extend to ranges from -3 to +3, and with further extensions, this range broadens to -4 to +4. These findings highlight the significant impact of extended NNN interactions on the topological properties of the two-leg-coupled SSH chains.

a0029

Interacting Grüneisen parameters in the spin 1/2 XX chain extended with three spin interactions

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We study the interaction dependent caloric effects in the exactly solvable spin-1/2 XX model in the presence of three-spin interactions of the XZX+YZY and XZY-YZX types. We introduce and compute novel 'interacting' Grüneisen ratios and study their dependence on the three spin interaction strengths. We show that interacting Grüneisen ratios not only capture the phase diagram but can also be used to characterize the nature of quantum phase transitions.

a0030

Evaluation of structural phase transition in spin-1/2 frustrated Dirac-magnon antiferromagnet: Cu_3TeO_6

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The topological magnonic lattice with quantum spins has been recently investigated in Cu_3TeO_6 both theoretically and experimentally. The quantum spins of Cu^{2+} (S = ½) in the cubic symmetry (Ia-3, a= 9.537Å) of Cu_3TeO_6 form low-dimensional geometry for instance non-coplanar hexagons and quasi-1D chains in a complex spin-web structure show interesting physical properties. We report the structural and magnetic properties by combination of *dc*-susceptibility, and temperature dependent x-ray diffraction as well as Raman spectroscopy over ultra-high quality single-crystals of Cu_3TeO_6. From recent ^{125}Te NMR measurements, a structural phase transition has been suggested by the emergence of new peaks in NMR spectra. However, we have performed a detailed x-ray diffraction and Raman technique to elucidate a structural-phase transition in frustrated spin ½ Cu_3TeO_6 compound, that the Cu_3TeO_6 undergo an isostructural transition with strong distortion in local octahedral environment, resulting in an unusually temperature dependence of cubic cell parameter and atomic displacement below the second-order phase transition (T_N = 61 K) which indicates strong magneto-elastic coupling. Our results reveal yet another interesting fact of the magneto-elastic coupling in the Cu_3TeO_6 spin-web lattice.

a0031

Dynamic Structure Factor of Warm Dense Homogeneous Electron Gas

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Warm dense matter (WDM) is an exotic state characterized by extreme densities, temperatures, and pressures, which is prevalent in nature, occurring mainly in astrophysical objects and brown dwarfs. Interestingly, it can also

be produced in laboratories using various techniques. The dynamic response property, such as the dynamic structure factor $S(q,\omega)$, is crucial for understanding the WDM critically, as it can be directly probed in x-ray Thomson experiments. Theoretically, this property is determined by the electron density's response to an external space-time dependent perturbation. In this paper, we report on the dynamic structure factor $S(q,\omega)$ of a warm dense three-dimensional homogeneous electron gas, which was determined using the finite-temperature version of the dynamical self-consistent mean-field theory developed by Singwi *et al*. Our results are compared directly with the recent ab-initio results of Dornheim et al., obtained using the path integral Monte Carlo (PIMC) simulations. Our study reveals that the static and dynamic local-field correction theories exhibit a reasonably good agreement with the PIMC simulations as compared to the random phase approximation. Our results underscore the significant impact of exchange-correlation effects on $S(q,\omega)$, as characterized by a red shift in the plasmon frequency with increasing coupling and its broadening at large wave vectors.

a0032

Effect of oxygen flow rate on thermochromic property of RF sputtered vanadium oxide thin films

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Vanadium dioxide (VO_2) exhibits insulator to metal phase transition (IMT) due to reversible change in carrier density which can be triggered by temperature, external or internal stress and doping etc. IMT results in change in optical and electrical properties of the VO_2 thin films. In this work, vanadium oxide (VO_x) thin films are prepared by of RF magnetron sputtering of VO_2 target at different oxygen flow rates. Distinctive change in color of the samples is observed when oxygen is introduced into the deposition chamber. The thermochromic properties of the deposited samples are investigated by measuring the resistance and transmission at different temperatures in the range of 30^0 C to 90^0 C. The resistance measurement shows that the thermochromicity increases by increasing the oxygen flow rate.

a0033

Construction of Optical Tweezers, Modelling, and Measurement of Optical Force

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Optical Tweezers are due to tightly focused laser beams created by using a high numerical aperture, capable of holding and manipulating microscopic particles in three dimensions [1]. Successful trapping of silica beads in the Newtonian fluid is achieved by using the Thorlabs OTKBM system. This work demonstrates the calibration of optical force and the factors that affect the optical trap. We will also explore the emergence of torque, windmill effect, and fluorescence on non-spherical objects.

a0034

High-Pressure behavior of Hexabromobenzene

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High pressure behavior of Hexabromobenzene (C_6Br_6) was studied using Raman spectroscopy up to ~23.8 GPa. Qualitative changes are noted in the Raman spectra around 6.1 GPa and 14.1 GPa indicating possible phase transitions in the compound at these pressures. Above 6.1 GPa, significant increase is observed in the intensity of CCC in-plane deformation mode at the expense of other Raman modes with broadening of all Raman bands over 22 GPa. Spectral features of HBB molecular unit persisted up to the highest pressure reached, namely 23.8 GPa.

a0035

Molecular Dynamics Investigation of Shock-Induced Phase Transition in Single Crystal Tungsten

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Extensive equilibrium molecular dynamics simulations are performed to investigate the shock Hugoniot behavior and dynamic structural response of single crystal tungsten (W) along three crystallographic orientations: [001], [110], and [111]. Our study reveals existence of strong crystal anisotropy in elastic-plastic two-wave region resulting in substantial variation in Hugoniot elastic limit and overdriven plasticity across three orientations. Further, shock-induced structural transitions from bcc to hcp and fcc phases are shown to initiate at 217 GPa and 232 GPa for [001] and [110] directions, respectively, whereas, [111] direction does not favor such phase transition. Notably, these transition pressures are significantly lower than those theoretically predicted hydrostatic compression-induced phase transformations at pressures exceeding 900 GPa.

a0036

Pressure induced changes in Biphenyl: A Raman scattering study

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High pressure behavior of the molecular crystal biphenyl studied by in-situ Raman spectroscopic technique upto 10 GPa is reported. Evolution of Raman spectra even at moderate pressure exhibit significant changes in the pressure dependencies. In particular, frequency of the inter-phenyl vibration and intensity of the C=C stretching vibration exhibit change in the pressure dependencies at pressure above 1.3 and 2.7 $\pm$0.4 GPa. Spectral changes are discussed in light of possible phase transitions in the system.

a0037

Structural Behaviour of $CaCu_4As_2$ under High Pressure

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A high-pressure study on $CaCu_4As_2$ was carried out using powder x-ray diffraction experiments. Our investigation shows that the ambient rhombohedral phase of $CaCu_4As_2$ remains stable up to ~ 42 GPa. These results are in contrast to the earlier low temperature studies where a structural phase transition was observed at 51 K associated with the formation of a charge density wave (1). $CaCu_4As_2$ shows the anisotropic compression with *c*-axis being the most compressible axis as a result of its layered structure consisting of $CaAs_6$ octahedra (L1) and $CuAs_4$ tetrahedra (L2) layers. We show that though the octahedra are more compressible than tetrahedra, the L2 layer consisting of tetrahedra shows more compression. The P-V data is fitted using a third order Birch-Murnaghan EOS which results in the bulk modulus, K_0 ~ 28.1 GPa and its pressure derivative K_0'~ 5.3.

a0039

High Pressure Study on Potassium Dicyanoargentate

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The Metal-Cyanide framework compound $KAg(CN)_2$ exhibits unusual behavior of vibrational modes under high pressure. High pressure spectra of the Metal-Cyanide compound observe the abrupt change in the vibrational mode frequencies in different pressure regions. Lattice and Bending modes were found to be blue shifting for all pressure values up to ~5.3 GPa beyond this low frequency modes could not be traced Ag-CN and CN stretching modes were found to be red shifted with pressure up to ~1.1 GPa accompanied with the splitting of CN stretching mode. First Principal Calculations suggest possible Negative Linear compressibility parallel to c-axis of the unit cell. To investigate the pressure induced response high pressure Raman study was carried out from ambient pressure to ~27 GPa. First principal calculations were carried out using projector-augmented wave (PAW) method through Vienna ab initio simulation package (VASP) to assess the vibrational and structural properties of $KAg(CN)_2$.

a0040

Pressure Induced Phase Transitions In (R-Ethylbenzylinium)$_2$CuCl$_4$ By Raman And X-ray Diffraction Study

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Pressure dependent Raman and X-ray diffraction measurements were carried out on (R-Ethylbenzylinium)$_2$CuCl$_4$-R-EBzCuCl: Chiral Organic Inorganic Hybrid Compound (OIHC). The high-pressure Raman analysis showed that the vibrations corresponding to organic moiety (i.e. Ethylbenzylinium group) developed and survived with increasing pressure due to which it surpassed the Jahn-teller (JT) distortion- the effect due to vibrations of inorganic moieties (i.e. $CuCl_4$). The phase change were observed at various pressures starting from 0.63 GPa, between 4.7-6.24 GPa and at 9.9 GPa. The *in-situ* powder X-ray diffraction analysis with pressure showed interesting changes with peak intensities and broadening, corroborating well with our high-pressure Raman analysis. The partial reversibility of the vibrational modes observed at full decompression suggested that the structural characteristics remained in-variant with pressure effect.

a0041

Weak Field Induced Spin-Correlation In $BaCo_2(As_{1-x}P_xO_4)_2$

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Honeycomb lattice materials have attracted great deal of interest as a Kitaev quantum spin liquid (KQSL) materials because of their high spin state and effective angular moment. $BaCo_2(AsO_4)_2$ is one of such compounds that crystallize with a rhombohedral structure (space group R-3) where Co^{2+} ions are located in a honeycomb lattice. In the present work we have studied effect of very low phosphorus substitution on As site in $BaCo_2(AsO_4)_2$ on polycrystalline sample using magnetization measurement. Temperature dependent magnetization shows decrease in antiferromagnetic ordering to 4.5K from T~5.4 K just by introducing 1% phosphorus. In doped sample, an intermediate magnetic state arises in the temperature window of 16K-20K as a hump in the magnetization measurement which is highly measurement history dependent and disappeared at very low magnetic field. Frequency dependent AC measurement also shows shift in transition temperature which support the existence of spin correlation well above the transition temperature in the present system.

a0043

High Pressure Raman Study of ZrV_2O_7 under Non-hydrostatic Condition

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ZrV2O7 has been investigated using Raman spectroscopy under non hydrostatic compression up to 10.2 GPa. Two transitions have been observed at 2.7 and 4.6 GPa respectively. Beyond 4.6 GPa gradual amorphization is observed in the compound. The transitions occurring at elevated pressures under non-hydrostatic conditions compared to hydrostatic compression indicates that ambient and high pressure structures remain more resilient in the presence of non-hydrostatic stresses. Our study further revealed that ZrV2O7 took distinct pathways for the pressure induced amorphization in hydrostatic and non-hydrostatic conditions.

a0044

Structural and Morphological Evolution of ZrO_2-Doped CeO_2 Under Xenon Ion Irradiation: Implications for Inert Matrix Fuel Applications

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This study investigates the effects of 1 MeV Xenon ion irradiation on $Ce_{0.75}Zr_{0.25}O_2$ with different grain sizes (Bm_1~300nm, BM_2~650 nm, BM_3~10 μm). The samples were synthesized using high-energy ball milling (HEBM) and characterized using X-ray diffraction (XRD), Raman spectroscopy, and scanning electron

microscopy (SEM). XRD analysis revealed peak broadening, intensity decrement, and peak shifting towards lower theta values with increasing ion fluence. The ion track diameters were calculated from relative lattice parameters, yielding values of (0.22±0.30), (0.44±0.68), and (0.63±0.71) nm for BM_1, BM_2, and BM_3, respectively. Raman spectroscopy showed redshifts in the B1g and F2g bands and blue shifts in the LO band, along with peak broadening at higher ion fluences. The ion track diameters, determined from the amorphous fraction, were (0.4±0.027), (0.811±0.034), and (1.076±0.027) nm for BM_1, BM_2, and BM_3, respectively. SEM analysis indicated an increase in grain size with higher ion fluences. The findings highlight the significant impact of ion irradiation on the structural and morphological properties of ZrO_2-doped CeO_2, with potential implications for advanced nuclear materials.

a0045

Probing of high pressure orthorhombic cotunnite phase in frustrated $Er_2Ti_2O_7$ pyrochlore titanate

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The structural stability of $Er_2Ti_2O_7$ cubic pyrochlore with pressure has been studied by photoluminescence, x-ray absorption and ab-initio calculations. From high pressure photoluminescence studies, a structural transformation was observed initiating at ~37 GPa. The high pressure phase is expected to have lower symmetry than the ambient pyrochlore phase. EXAFS measurements were performed at Er^{3+} edge on the recovered sample and compared with the pyrochlore phase. The analysis suggests increase in coordination from eight to nine due to the phase transition. From DFT based first calculations, it was found that cotunnite phase becomes energetically more stable than ambient pyrochlore phase at ~53 GPa. Therefore the high pressure phase has been predicted to be orthorhombic cotunnite phase which is a highly disordered phase where both the cations and anions are randomly distributed on 4c positions and one eighth of the oxygen atoms are missing. Theoretical P-V data has been fitted with the third order BM EoS and obtained values of B and B' for pyrochlore structure are 189 (12) GPa and 4(3) respectively. Similarly, for the high-pressure cotunnite phase the corresponding values are 168 (10) GPa and 5(2) respectively. It suggests that the high-pressure phase is more compressible than the pyrochlore phase.

a0046

Hexagonal to Orthorhombic Phase evolution in Ho doped $LuFeO_3$ multiferroic

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$LuFeO_3$ is an attractive material as it exists in hexagonal and orthorhombic phases and exhibits corresponding ferroelectric and magnetic properties. The material is well studied in its orthorhombic phase while the metastable state is explored. The polycrystalline Ho-doped $LuFeO_3$ samples are prepared using the sol-gel synthesis method, and a phase evolution from the metastable hexagonal to orthorhombic phase is observed as Ho doping content increases in Lu- site of $LuFeO_3$. The XRD shows the orthorhombic phase as an impurity in the hexagonal phase, which is the corresponding change in the lattice parameters, crystal distortion, and bond lengths that affect electric and magnetic properties.

a0047

The Effect of Pressure on ZIF-67: An X-ray Diffraction and Infrared Study

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ZIF-67 is a porous material in the family of zeolitic imidazolate frameworks (ZIF) having structural similarities with technologically important ZIF-8 compound. The structural stability of these compounds is of great significance for a wide range of practical applications. Here, the structural details of ZIF-67 bulk powder perturbed by external pressure have been thoroughly investigated utilizing synchrotron based X-ray diffraction and infrared spectroscopy techniques. ZIF-67 exhibits a reversible phase transformation upon decompression from a partially disordered state, while using a penetrating pressure transmitting medium (PTM). This is in contrast to the earlier report suggesting an irreversible transformation upon decompression, carried out using non-penetrating PTM or without any PTM. Pore gate of 4-MR opens at 2.7 GPa in our case, accompanying the rotation of 2-MEIM linker chains by around 20°. We have also observed a complete collapse of framework structure around 13 GPa

associated with change in colour from light violet to purple. Thus, this study sheds light on the available mechanical modifications and selectivity targetted applications of ZIF-67 as gas absorbents.

a0048

Calculation of Gruneisen parameter for Al and Mg up to 150 GPa employing Shock data

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First, Hugoniot pressure and energy of Al and Mg up to 150 GPa has been evaluated using shock-particle velocity experimental data. Then, the Gruneisen parameters (Γ (V)) have been computed at different volumes employing Birch-Murnaghan equation of state (EOS) and four parameter EOS in Mie-Gruneisen EOS along with the above Hugoniot pressure and energy. For both elements, initially the parameter increases and then decreases monotonically with compression. Here, the behavior of Γ(V), obtained from shock experiment, is not monotonous and it differs from earlier proposed models. Hence Mie-Gruneisen EOS cannot be employed to determine Γ(V) directly from shock wave data.

b) SOFT MATTER INCLUDING POLYMER AND BIOLOGICAL SYSTEMS

b0004

Highly Transparent Heat-Induced Gels of Nanoparticle-Protein Dispersion

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Nanoparticle-protein systems gathered huge scientific interest due to the synergistic effects of nanoparticles and proteins useful for vast applications in the field of nanobiotechnology. The interaction between the two components in their dispersion with respect to different physiochemical parameters is being widely studied, however, investigations guiding their gelation are still required. In this work, we present a pathway of fine tuning the interaction between nanoparticle and protein in dispersion to achieve their gels with tunable properties. These gels are prepared by heating the dispersion of anionic silica nanoparticles and anionic bovine serum albumin protein in suitable concentration ratio, beyond a critical gelation temperature (TG). The proteins undergo hydrophobic attraction to form a 3-dimensional gel network, where presence of nanoparticles introduces additional electrostatic repulsion. The interplay of these two interactions decides the physical properties of thus formed gels. The nanoparticle-protein gels are highly transparent (transparency ~ 85%) compared to the gels of the pure protein (transparency < 1%) while their strength depends on the relative concentration of the nanoparticles, leading to the formation of tunable hard and soft gels. Such transparent gels with tunable strength can possess a range of applications such as in contact lens, imperceptible soft robotics and invisible wearable devices

b0007

Preparation And Magneto-Structural Characterization Of Hyaluronic Acid-Coated Iron Oxide Nanoparticles For Optimized Magnetic Fluid Hyperthermia

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This study investigates magnetic fluid hyperthermia properties of hyaluronic acid-coated iron oxide nanoparticles (HA-MNPs). The HA-MNPs, with a size of ~11.7 nm, are prepared using a co-precipitation technique, followed by ligand exchange. The synthesized HA-MNPs exhibit good colloidal stability (hydrodynamic diameter: ~19.5 nm and a zeta potential of ~ -24.3 mV). The saturation magnetization and blocking temperature of the HA-MNPs are found to be ~ 59.3 emu/g, and ~ 175 ± 2 K, respectively, indicating the superparamagnetic nature of the prepared MNPs at room temperature. Magneto-calorimetric studies show superior field-induced heating efficiency of the HA-MNPs, where for MNP concentrations of 2-5 wt. %, the temperature rise is found to exceed the threshold (~ 42 ^{o}C) for magnetic fluid hyperthermia. Immobilization of the MNPs in a tissue equivalent agar matrix is found to reduce the heating efficiency due to the abrogation of Brownian relaxation. Orientational ordering of the MNPs under an external DC magnetic field aligned parallel to the AC field is found to increase the heating efficiency due to an enhancement in the effective anisotropy energy density.

b0008

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

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We present a study of comparative translation dynamics of 1)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 and 2) the Kob-Anderson 80-20 mixture. A comparison of the relaxation times of these two models shows that the FENE dumbbell molecular liquid has faster dynamics than the standard Kob-Anderson model despite the heavier molecular weight of the former, thus showing reduced dynamic heterogeneity.

b0009

Temperature-Dependent String-Like Cooperative Motions in Kob-Andersen Binary Mixtures

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Abstract. This study investigates the probability distribution of string sizes in a Kob-Andersen particle mixture under varying temperatures. We study the influence of temperature on string formation by molecular dynamics simulations of the Kob-Andersen binary mixture. Our results reveal that smaller strings are more probable at lower temperatures, while higher temperatures lead to a more uniform distribution of string sizes. The probability decreases exponentially with increasing string size, highlighting significant temperature-dependent structural changes in the system. These findings provide deeper insights into the dynamics and interactions within particle mixtures, contributing to the broader understanding of complex systems.

b0010

Nonequilibrium Work Fluctuations in Force-induced Melting of a Short B-DNA

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A system of a solvated canonical B-DNA of 12-base pairs with the specified sequence is initially equilibrated in a state of zero external force f acting on it. After equilibration, a switching experiment is performed over the system by pulling one end of the DNA while restraining its other end. The finite time pulling process is performed at a constant rate of the applied force, until a maximum value of $400\ pN$. The associated nonequilibrium work done (W) during this process is determined by numerically integrating the force-extension curve, as a function of the applied force. An ensemble of the work values, $p(W)$ is obtained by repeating the pulling experiments a large number of times. The free energy difference (ΔF) between the equilibrium and force-induced melted states of the DNA is determined by employing the Jarzynski equality. The value of ΔF is found to be in close agreement with the conventional equilibrium methods

b0011

The Effect of Monomer Concentration Variation on the Rheological Properties of the Agar- Polyacrylamide Double Network Hydrogel

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A physically-chemically cross-linked combined agar-polyacrylamide double network hydrogel was prepared utilizing one pot method via heating- cooling photo polymerization method. The rheological properties of the prepared gel were investigated by varying the concentration of the Agar, the first network, while keeping the second network, PAM, concentration constant and vice versa. The linear viscoelastic region (LVR) of the sample was determined from amplitude sweep measurements. The order of the elastic components was found at least two orders of magnitude more than the viscous components. The gel strength increased with the increase concentration of both the network.

b0012

Incorporated Polyelectrolyte Chain Effects on the Rheological Properties of Polyacrylamide Hydrogel with and without Monovalent Salt

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In the current study, we have studied the effect of entrapped polyelectrolyte chains of NaPSS on the viscoelastic behaviour of the gels in the presence of monovalent salt using rheological measurements. It is seen that the storage modulus G' depends on the non-gelling polymer concentration. With the increase of NaPSS concentration, the storage modulus of gels gradually decreases, weakening the gel strength. However, with the addition of a monovalent salt of NaCl, the gel de-swells and improves the mechanical strength of the samples.

b0015

Active Rod Inside A Rigid Ring Exhibits Non-Monotonic Tracer Dynamics

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Self-propelled objects refer to biological entities that consume energy from the environment or utilize their internal chemical energy to generate directed motion. We study the behavior of self-propelled rods in two dimensions, confined in a rigid ring using Langevin dynamics simulations. To investigate the dynamics of the rods, we measure the number of unique visits made by the rod in the circular confinement with varying Peclet number (Pe). For the passive rod with a lower value of Pe, we observe that the rod explores central as well as the peripheral regions. As we increase the active force of the rod, at intermediate Peclet number the rod exhibits only the peripheral region of the confinement. Counterintuitively, if we further increase the Pe, the rod again starts to exhibit both the bulk and peripheral motion, a similar trend of motion as for the lower Pe. To elucidate the dynamics, we compute the Mean Squared Displacement (MSD) of the rod. Contrary to common belief, though the MSDs are monotonically increasing with Pe, the nature of the trajectory is switching between the localized peripheral and diffusive bulk motion, which we finally quantify by measuring the unique block visit.

b0016

Small Angle Neutron Scattering Study of Hydrophobic Silica Aerogels

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Small angle neutron scattering is well established method to probe nanostructures. Nano structural silica aerogels were synthesized by ambient pressure drying method. Amorphous nature of the aerogel is confirmed by x ray diffraction. Fractal structure of the aerogel has been observed which arise as a result of aggregation and the synthesis condition. Fractal dimension was found to vary from 2.35 to 2.87 indicating highly porous nature of aerogel. With increase in surfactant concentration the correlation length (ξ) increased from 140 to 300nm.

b0017

A Study of the Effect of High Energy Radiation on Polyolefin/Natural Fibre Composite

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Natural fibre reinforced polyolefin composite has attained great attention in the last few years. Flax fibre is an attractive and potential fibre for preparation of polymer based partially bio-degradable composites to reduce the microplastic pollution. However, preparation of such composites with desired properties is a challenge due to the dissimilar surface wettability (surface energy) of polyolefin and flax fibre. In this work, we report hydrophobic surface modification of flax fibre to make it similar to polyolefin in terms of surface wettability. Composites of pure flax fibre and modified flax fibre with linear low density polyethylene (LLDPE) have been prepared. Pure and modified fibre incorporated composites are thoroughly studied. Prepared composites are irradiated at different EB doses using an electron beam (EB) accelerator. Improvement of mechanical and dynamic mechanical properties are found higher in case of surface-modified flax fibre incorporated composites than pure flax fibre based composites of similar loading. The properties are improved more upon electron beam irradiation.

b0018

Preparation of LLDPE/Starch Composites by High Temperature Processing Overcoming Persisting Challenges

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There are many challenges in preparation of filler reinforced composites such as poor mechanical properties of the prepared composites, less filler-containing capability of polymers, poor processability of high filler-containing composites and compromised mechanical properties of prepared composite. To overcome these challenges, we have melt blended ENGAGE, with LLDPE and modified starch. ENGAGE creates space in the LLDPE/ENGAGE blend to accommodate high quantity of starch. Up to 70 wt% starch is able to incorporate in polyolefins. Also, due to unique processability of ENGAGE, it improves the processability of high starch containing LLDPE composite. Mechanical properties of starch incorporated composites are thoroughly studied. The Young's moduli of composites are improved and elongations are maintained at a considerable value. Thermogravimetric analysis (TGA), scanning electron microscopy (SEM), rheological and dynamic mechanical analysis are carried out to establish structure property

relationship. Polyolefin composite with 70 % of biodegradability and around 230 % elongation is unique and useful many applications especially in packaging.

b0019

***In-situ* Fabrication Of ZnO@PVA Nanocomposite Film: A Flexible Free-standing Film With Antimicrobial Activity**

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Herein we fabricate flexible free-standing poly(vinyl alcohol)-zinc oxide (PVA-ZnO) nanocomposite film using simple solution casting technique. The formation of ZnO nanoparticles (NPs) was confirmed by X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Mechanical properties and antimicrobial activity were evaluated by analyzing stress-strain plots and observing the zone of inhibitions on the Meuller Hilton agar plates respectively. The results demonstrated that PVA-ZnO nanocomposite films exhibit excellent flexibility of 645%. The nanocomposite film shows significant antimicrobial activity against Gram-negative and Gram-positive bacteria and fungal pathogens. These finding indicates that the nanocomposite films could be used as packaging materials and antimicrobial coatings

b0020

Cholesterol-induced Modification in Lysozyme-DMPA Mixed Langmuir Monolayer

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Langmuir monolayer of pure cholesterol, lysozyme-DMPA (LyD) and cholesterol-lysozyme-DMPA (CLyD) are formed on the aqueous subphase having pH ≈ 7.0. To investigate the effect of cholesterol on the phases and phase transition occurring with monolayer compression, Surface pressure (P)-mean molecular area (A) isotherms are recorded from all three monolayers. P-A isotherm reveals a distinct behavior of the CLyD monolayer than that of the LyD monolayer, with the occurrence of plateau region and collapse point comparatively at lower P. The morphological feature captured from BAM at P ≈ 30 mN/m shows a more compact structure of the CLyD monolayer than that of the LyD monolayer, causing the more stable nature of the CLyD monolayer at the same P

b0021

Statistical Properties of Passive, Self-Propel and Janus Particle in Ordered Crowding

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Transport of single molecules via passive or active processes are crucial for the functioning of biological systems. Statistical physics models are useful in understanding the underlying physical mechanism of such systems. In this study, we have discussed a comprehensive study on how activity plays a crucial role in the dynamics of passive, active, and Janus particles inside non-inert ordered crowded environments. We designed the system in the underdamped limit with sticky crowders to make the scenario a biologically relevant environment having high damping with attractive centers. Our main objective here is to elucidate the dynamics of active and passive particles as the effect of stickiness and packing fraction of the crowders. The passive particle shows sub-diffusion and the self-propelled particle shows super diffusion despite being obstructed by crowders. Due to the presence of the ordered attractive centers, in the intermediate value of the packing fraction shows counterintuitive maximum diffusive behavior. Further, the strength of the active force can nullify the hindering effect of sticky crowders on the diffusion constant. In addition, we studied the dynamics of Janus particles.

b0022

Percolation/Relaxation Behaviour Of Cold Pressed PVDF/$CoFe_2O_4$ Polymer Nanocomposites

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The cold-pressed polymer nanocomposites **(**PNC) of PVDF and $CoFe_2O_4$ (prepared through the co-precipitation method) were prepared with the help of a hydraulic press at room temperature under 10MPa. The PNC was characterized for structural, micro-structural & Dielectric properties respectively. Rietveld refined XRD confirmed the phase formation of $CoFe_2O_4$ and the micro/nanostructures were found from FESEM images. The percolation behaviour of the PNC is observed at a percolation threshold of f_c=0.3, which is associated with an insulator-to-metal transition (IMT) behaviour & the enhancement dielectric parameters were explained using the MWS/interfacial polarization. The scaling laws for explaining the IMT behaviour of PNC were implemented and the universal scaling exponents [s, s' & t] were obtained. Also, the non-Debye relaxation behaviour was found with the help of Jonscher's law for all the samples at both sides of IMT.

b0023

Cloning, Expression, Purification and Crystallization of Ribosomal-Protein L7/L12 from *Mycobacterium tuberculosis*

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Tuberculosis is a fatal disease caused by *Mycobacterium tuberculosis* with high rate of relapse and mortality worldwide. Stalk protein L7/L12 from *Mycobacterium tuberculosis* is a part of 50s ribosomal subunit, involved in translational process during protein synthesis. In this study, the L7/L12 ribosomal gene of *Mycobacterium tuberculosis CDC1551* was cloned into prokaryotic expression vector pET28A, then expressed, purified and crystallised by vapor diffusion method. Crystals of L7/L12 were obtained in 0.1 M Ammonium acetate pH 7.0, 25% PEG 8000, 25% Ethylene Glycol at 20°C. Diffraction data at 100 K was collected at inhouse Excillium Metal Jet X-ray Diffraction system. L7/L12 protein crystallized in *P22121* space group with unit cell dimension of a=25.86, b=47.27, c=61.07, and $\alpha = \beta = \gamma = 90°$. The mathew's coefficient and solvent content was found to be 2.45 and 49.74% respectively. Due to its importance in the translational process its structural and function knowledge is essential to understand the translational biology and can be a potential for drug development.

b0024

SANS study of polymer induced modifications in structure and interactions in Water/AOT/Dodecane Microemulsion Droplets

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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 polymer strength and concentration play crucial role in tailoring the structure and interactions of the droplets. The complex role of polymer in stabilization of these droplets and modifications of structure and interaction through change of inter-droplet interfacial potential is elucidated using a sticky hard sphere potential with mean spherical approximation. It has been shown that the stability of droplets decreases with increasing polymer concentration, whereas it is more or less independent of the molecular weight of the polymer.

b0025

Exploring the Free Energy Landscape of a Structurally Homologous Protein using Replica Exchange Molecular Dynamics

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The topology of the free energy landscape of proteins is key to understanding various biochemical processes. The rugged nature of a protein's free energy landscape makes it challenging to explore its entirety using biomolecular simulations. In this work, we studied the unfolding of structural homologs of an enzyme known as acyl-phosphatase and employed Temperature-Replica Exchange Molecular Dynamics to investigate their free energy landscapes. The analysis of intra-molecular contact maps and hydrogen bond fractions during the dynamics reveals how protein sequences encode their free energy landscapes.

b0027

Micro-scale Dynamics in Disordered Polymers and Gels Influences Macroscale Response

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A comparative experimental analysis of dynamics at the micro-scale is presented for polymer glasses and gels. These are disordered, off-equilibrium systems, with physical properties showing time evolution, non-Gaussian fluctuations, or jammed, heterogeneous dynamics. We show how these micro-scale dynamics affect the macroscopic properties of these systems. In the case of polymers, glassy dynamics at the micro-scale is shown to influence the macroscopic tensile response. There is a presence of caged β relaxation dynamics, in addition to α-relaxation. On the other hand, in gels, the mechanism of drug release is found to be affected by the micro-scale diffusion, measured with fluorescence recovery after photobleaching, and macro-scale diffusion, measured through release kinetics of a fluorescent molecule. Both the macro-scale and micro-scale properties are observed to be influenced by the gel network structure, which has a slow ageing dynamics.

b0028

Miscibility, Compatibility and Intermolecular Interaction Analysis of Oxypropylene Blends with Isobutene and Acrylonitrile

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A compatibility study was conducted on polymer blends comprising oxypropylene as the base polymer with isobutene and acrylonitrile as screen polymers. Thermodynamic parameters, including Flory-Huggins interaction parameter (Chi), mixing energy (Emix), and average interaction energies, were calculated at 298 K. Results indicate poor compatibility between oxypropylene and isobutene, as evidenced by a high Chi value of 0.73326731. In contrast, the oxypropylene-acrylonitrile blend exhibited relatively better compatibility with a Chi value of 0.13832991. Oxypropylene and acrylonitrile exhibit better compatibility compared to oxypropylene and isobutene.

b0029

Structure and phase transitions in Lipoplexes

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Gene therapy is an emerging therapeutic approach that aims to treat diseases by delivering genetic material into cells. Due to the inherent challenges of delivering naked deoxyribonucleic acid (dna) into cells, cationic liposomes have become a preferred method. In this study, we aim to investigate the structure and phase transitions of synthetic cationic dioctadecyldimethylammonium bromide / dna lipoplexes at varying charge ratios. Our dynamic light scattering and zeta potential measurements suggest that the presence of dna does not significantly affect the size of the lipoplexes in negatively and positively charged regions, while it leads to lipoplex aggregation in the neutral region. Differential scanning calorimetry and fourier-transform infrared spectroscopy results indicate that in the positively charged region, the presence of dna induces two phase transitions: one associated with the excess liposomes and the other with the formation of lipoplexes. As the dna concentration increases, approaching the neutral region, a single transition is observed, suggesting that nearly all liposomes are involved in lipoplex formation.

b0030

Ubl Domain: A key Player in SARS-CoV-2 PLpro Structure and Function

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Papain-like-protease (PLpro), a part of SARS-CoV-2 Nsp3 domain, essentially has two sub-domains, a N-terminal Ubl domain and a well separated catalytic core domain. The role of Ubl domain in PLpro structure and function is not yet clearly understood. Here, in our study we have expressed, purified and thoroughly characterized PLpro without the Ubl domain (Truncated PLpro). We found that the PLpro without Ubl domain is able to cleave the RLRGG-AMC, Ub-AMC and ISG15-AMC substrates but at a much lower efficiency than wild-type. There is an inherent instability and susceptibility to aggregation in Truncated PLpro which may be attributed to the absence of initial sixty residues which although are away from the catalytic site, but still might be important for substrate binding and overall stability of PLpro. The ability to convert pro-ISG15 to m-ISG15 has also been studied. We have crystallized both the proteins and the structure is discussed. Therefore, Ubl domain is important for the functional and structural stability of PLpro protein.

b0033

Electronic and Optical Characterization of Polypyrrole Thin Films: A UV -Visible Absorption Study

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The Polypyrrole is a heterocyclic and positively charged conducting polymer (CP) that contains nitrogen in its oxidized form, and it loses its conductivity and charge when overoxidation occurred. Its exceptional electrical conductivity, chemical stability, high surface area and sensitivity to environmental changes makes it ideal for gas sensing applications. In this study, polypyrrole is synthesized by chemical oxidative polymerization of Pyrrole monomer and ammonium persulfate as oxidant in different ratios. Polypyrrole thin film is cast by dip coating technique. The electronic transition is analyzed for various oxidant concentrations and absorption peak at about 450 nm corresponding to the π-π* transition. Band gap of samples is found in semiconducting range. Optical constants such as absorption coefficient, extinction coefficient, refractive index and optical conductivity have been evaluated for all the samples and have been studied as a function of energy.

b0034

Recycling of Medical Face Mask waste to an Engineering Materials: A study on the Nonwoven Polypropylene Nitrile Rubber Blend

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This study turns used face mask garbage into a useful resource, addressing the environmental problem associated with it. Every day, billions of single-use face masks are used worldwide, hence the COVID-19 pandemic has an influence on waste management. It might be difficult to dispose of used face masks properly without putting the environment or human health in jeopardy. This article investigates a cutting-edge method for reusing medical face masks. Using maleic anhydride as a compatibilizer, nonwoven polypropylene (PP) fiber from masks is combined with acrylonitrile butadiene rubber (NBR) to create a PP−NBR blend. Sterilized waste was examined for pathogens, followed by characterization using differential scanning calorimetry (DSC), Fourier transfer infrared spectroscopy (FTIR), and thermogravimetric analysis (TGA). An in-depth study of the blends' mechanical, thermal, and biological properties showed improved thermomechanical properties, with 50 wt% PP.

b0035

Butyl Rubber Based Chemiresistive Sensor for Room Temperature BTEX Sensor

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Benzene, toluene, ethylbenzene, and xylene, collectively known as BTEX, are aromatic hydrocarbons widely employed in the petrochemical, agrochemical, and pharmaceutical sectors. Despite their industrial significance, these compounds pose substantial health risks, including carcinogenicity. Consequently, the development of rapid and reliable monitoring methodologies is imperative. Conventional BTEX sensors suffers from the limitations such as high temperature consumption. Butyl rubber/CNT nanocomposite has shown chemiresistive behaviour in presence of aromatic VOCs. However, due to its high molecular weight solubility is less and hence the sensitivity. We employed controlled radiation induced degradation at 10kGy radiation dose to achieve improved chemiresistive sensitivity towards BTEX compounds.

b0036

Influence of Electric Field on Protein Phase Behavior

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We examined how an externally applied electric field affects protein crystallization, liquid-liquid phase separation (LLPS), and crystallization kinetics. Under a weak alternating current (AC) electric field, crystallization occurs over a broader region of the phase diagram, nucleation induction times decrease, and crystal growth rates increase. Conversely, LLPS is suppressed, reducing the likelihood of a two-step crystallization process. The electric field's effect is attributed to a change in the protein-protein interaction potential.

b0037

Development of Sustainable Absorbent Wheat Gluten-Based Composition: Evaluation of Properties

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The current research implies the development and its property evaluation of bio-based wheat gluten foam (WGF) absorbent material preferably suitable for hygiene application. Here, WGF foam exhibits an increased absorbency value in various liquid mediums including distilled water, 0.9wt.% saline solution and defibrinated sheep blood media. As, the mechanical stability of the neat WGF (S1) was decreased after liquid immersion, Gallic acid (GA) and Bagasse fibre powder (BFP) were used as a bio-based crosslinker and a reinforcement, respectively to enhance its properties. The presence of only gallic acid in the foam (S2) showed absorbency of 7.8 g/g in distilled water, 9 g/g in saline and 6.3 g/g in sheep blood at 240mins with some structural disintegration. On the other hand, the combination of BFP and GA-based wheat gluten foam (S3) showed absorbency of 8.9 g/g in distilled water, 9.4 g/g in saline and 6.5 g/g in sheep blood at 240mins time duration without disintegration. Absorbency under load test and compressive test were performed for all samples, in which S3 showed better blood absorbency of 7.5 g/g and also possessed better compressive strength of 0.35 MPa at a strain of 0.012. Through Scanning electron microscopy (SEM), the porous structure of every sample was identified and around 79.863% of open cells present in the S3 composition were identified by gas pycnometers. The soil burial test was carried out to analyze the degradation behaviour of the developed samples. Additionally, they showed better thermal stability confirmed by thermo gravimetric analysis (TGA). Thus, these findings revealed the cost-effective development of a sustainable absorbent composition, which may find effective use in hygiene applications.

b0038

Comparative Infrared Spectroscopic Studies of Mitochondrial targeting Curcumin Derivatives

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Curcumin has now been seen as a wonder drug due to a range of therapeutic benefits. However, to address the challenges linked to its clinical applications, which are limited by water insolubility and low bioavailability, first step is the accurate determination of molecular structure. Curcumin possesses three intramolecular hydrogen bonds close to its binding sites, one of which shows high proton delocalization. Very recently, the synthesis of mitochondria-targeted curcumin (mitocurcumin, MC), has been reported by conjugating curcumin to triphenylphosphonium cation, which has shown many fold increase in the efficacy of curcumin. With this strategy, the OH groups at the edges of molecule are replaced by triphenyl phosphine groups (one in MC2 and both in MC1). Here, we present the first vibrational spectroscopic characterization of MC1 and MC2 alongwith UV-Vis spectroscopic results, to compare their molecular structure, bond strengths and nature of hydrogen bonding interactions with that of curcumin. Our results show that MC1 shows significant difference in molecular geometry as well as hydrogen bonding interactions than pure curcumin and MC2, thus explaining the reasons for its superior biological properties.

b0039

Optimal Transport conditions of a Run and Tumble Particle in a Ratchet potential

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Using Brownian Dynamics simulations we explore the optimal transport conditions of a run and tumble Brownian particle moving in an asymmetric piece-wise linear ratchet potential. The particle current can be optimized with respect to the self-propelled velocity of the run and tumble particle as well as the temperature of the thermal bath and the asymmetry parameter of the potential. However, the unidirectional motion of the particle is executed in an incoherent manner as shown by low values of the Peclet number. Additionally, the net current as well as the diffusivity degrade with the increase in the rate of tumbling events as frequent changes in orientation traps the particle at the minima of the potential.

c) NANO-MATERIALS

c0002

Synthesis and Characterization of Anatase Phase Nanocrystalline-TiO_2 by Hydrothermal Method

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Titanium dioxide (TiO_2) nanoparticles show great promise for environmental remediation due to their photocatalytic properties and non-toxic nature. This study explores the hydrothermal synthesis of nanocrystalline TiO_2 powder with a dominant anatase phase, known for its high photocatalytic efficiency. The synthesis used a hydrothermal reaction of titanium isopropoxide with Acacia gum, followed by calcination at 500°C. Characterization through Transmission Electron Microscopy (TEM), X-ray Diffraction (XRD), and Raman Spectroscopy confirmed a particle size of 20-50 nm and the predominance of the anatase phase. TEM images showed well-dispersed nanoparticles, XRD revealed mainly anatase with minimal rutile, and Raman spectra confirmed the anatase structure. Zeta potential measurements across pH 3-10 showed a high positive zeta potential at acidic pH and a stable negative zeta potential in alkaline conditions, indicating better adsorption in alkaline environments. This study highlights the effectiveness of hydrothermal synthesis for high-quality TiO_2 nanoparticles and their potential for environmental cleanup, particularly arsenic removal from water.

c0003

Augmented field emission properties from MoO_3 rods derived via chemical route

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Here, we have synthesized the monoclinic phase of MoO_3 by using the micellar route. Structural analysis of MoO_3 shows the formation of monoclinic molybdenum oxide (MoO_3). Transmission electron microscopic studies of MoO_3 reveal a nanorod-like morphology having a diameter of ~100-200 nm, and a length of ~500 nm-1μm, further, the obtained MoO_3 was spin-coated over n-type silicon substrate, and field emission study of MoO_3 film was investigated. The observed field enhancement factor (β) and turn-on field of MoO_3 were 1.9×10^3 and 3.30 V/μm. The current study opens up new avenues for the affordable and scalable usage of MoO_3, to be employed as an electron emitter in a high-end optical and electrical device.

c0004

Structural, Magnetic, and Raman Analysis of Strontium-Doped Nickel-Zinc Nano Ferrite

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Over the past few years, significant advancements have occurred in both technology and scientific understanding within the field of nanomagnetism, particularly in Nickel-based nanoferrites ($NiFe_2O_4$), due to their unique physical and chemical properties.

The present study is focused on structural, magnetic and Raman study on Strontium doped Nickel-Zinc Nano Ferrite (NZSFO). For this modified cost effective sol-gel technique is adopted. The structural analysis revealed that the synthesized NZSFO ferrite formed as a single phase and cubic spinel structure with Fd-3m space group. Using Rietveld refinement, the lattice constant and by Debye Scherrer formula, strain and crystallite size were estimated. There is an increase in the lattice constant and decreases in the crystallite size. The M-H hysteresis curve recorded at room temperature using the Vibrating Sample Magnetometer (VSM) technique. The data revealed an increase in saturation magnetization and a decrease in coercivity, indicative of super-magnetic behavior. Raman spectra displayed five Raman modes (A_1g, Eg, and $3F_2g$), confirming the purity of the samples. These properties make the material suitable for applications such as data storage and magnetic tape recording.

c0006

Tailoring the Structural and Magnetic Properties of $SrBi_2Nb_2O_9$ through $ZnFe_2O_4$ Incorporation

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The $SrBi_{2-X}(ZF)_XNb_2O_9$ (where X = 0.0 - 0.5 with a step size of 0.1; ZF= $ZnFe_2O_4$) nanocomposite with a dual-phase crystal system of ($A2_1am$) and (Fd-3m) were synthesized from the hydrothermal method. X-ray Diffraction confirms Orthorhombic structure in $SrBi_2Nb_2O_9$ (SBN) and Orthorhombic-Spinal structure in the composite materials upon the introduction of ZF in the host SBN matrix. Rietveld analysis of XRD data showed a change in lattice parameters and cell volume. A profound impact of ZF on SBN was noticed in the VSM study. The enhanced magnetic saturation values and squareness parameters make the studied materials promising candidates for memory devices (NVRAMs) applications.

c0007

Chemical Synthesis, Characterization And Magnetic Properties Of $NiLa_xFe_{2-x}O_4$ ($0 \leq x \leq 0.3$) Nanoparticles

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By using sol gel autocombustion technique, synthesis of lanthanum (La^{3+}) substituted nickel ferrite nanomaterial ($NiLa_xFe_{2-x}O_4$, $0 \leq x \leq 0.3$) has been achieved. Materials characterization were carried out using powder XRD, FESEM, Raman spectroscopy and magnetic measurements. The materials crystallize in cubic structure having lattice parameters of 8.3269 Å, 8.3288 Å, 8.3340 Å for La content, x = 0.0, 0.1 and 0.3 respectively. The calculated crystallite sizes decrease from 42 nm down to 29 nm for $0 \leq x \leq 0.3$. FESEM studies confirm spherical nature of the particles with particle sizes of 40 nm, 28 nm and 33 nm for x = 0.0, 0.1 and 0.3 in $NiLa_xFe_{2-x}O_4$, respectively. Metal-oxygen bonds in various tetrahedral and octahedral sites were examined by Raman spectroscopic technique. The values of saturation magnetization, M_s and coercivity, H_c, can be tuned as a result of gradual increase in lanthanum content (x) in $NiLa_xFe_{2-x}O_4$.

c0008

Exploring the Structural and Magnetic Properties of Cu-doped $NdFeO_3$ Orthoferrite

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We prepared Cu-doped $NdFeO_3$ using the sol-gel citrate technique and studied its structural and magnetic characteristics. Rietveld refinement of the samples demonstrated strong alignment between experimental and theoretical X-ray diffraction (XRD) findings, affirming effective refinement and confirming that the samples exhibit orthorhombic crystal symmetry within the Pbnm space group. The introduction of Cu at Fe site resulted in an expansion of the unit cell volume and lattice parameters (a, b, and c), attributed to the larger ionic radii of the substituted ion. Simultaneously, the average crystallite size decreased with higher doping concentrations, as calculated by both the Debye-Scherrer method and the Williamson-Hall analysis. At room temperature, $NdFeO_3$ exhibits strong antiferromagnetism with a weak ferromagnetic contribution due to Dzyaloshinskii–Moriya (D-M) interaction. Cu doping at Fe site strengthens the overall magnetization.

c0009

Structural and Optical Properties of Ni-doped ZnO thin films Synthesized by Sol-gel Spin coating method

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This work examines the impact of transition metal (TM) substitution on the structural and optical properties of $Zn_{1-x}Ni_xO$ (x = 0, 0.1) thin films that are formed onto ITO substrates using the sol-gel spin coating method. Zinc acetate dehydrate, 2-methoxy ethanol, and ethanolamine were used as the precursor, solvent, and stabilizer, respectively. The mixture was doped with nickel (II) acetate tetrahydrate. Hexagonal Wurtzite structure is evident in all of the thin films according to X-ray diffraction patterns. The lattice parameter 'a' and 'c', volume and bond length of Ni-doped ZnO thin films slightly more than that of pure ZnO nanoparticles. The crystallite size decreases as doping. The optical transmittance of the synthesized film measured between 350 and 800 nm in wavelength range, and their band gap is determined. From the Optical UV-Vis studies, it is evident that the transmittance value increased as the concentration of a dopant fraction increases. The optical band gap of the synthesized thin films lies between 3.245–3.663 eV.

c0010

Optical Characterization of Hydrothermally Synthesized Quantum Dots: Insights and Analysis

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Abstract. This study reports the successful fabrication of carbon quantum dots (CQDs) from milk through hydrothermal technique. No specialized tools or chemicals are required for a straightforward and environmentally safe process. The CQDs were approximately 7 nm in size and exhibited a nearly circular shape upon synthesis. Their primary components included nitrogen, oxygen, and carbon. They display temperature-dependent photoluminescence and broad excitation-emission spectra. They remained pretty stable with their storage time. The selective and sensitive response of luminescence quenching mechanisms makes them suitable for developing a nanosensor to detect Sn^{2+}.

c0011

In-modified ZnO Nanowires based NO Sensor

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We report a low-temperature, high-performance NO gas sensor based on indium (In) modified ZnO nanowires (In-ZnO NWs). The 'In' was deposited on the NW's surface using the thermal evaporation process. XRD and SEM-EDS analysis of In-ZnO NWs revealed that the produced ZnO NWs have a hexagonal structure with 'In' dispersed on the surface. Gas sensing studies revealed that In-ZnO NWs had a stronger response, a lower ideal operating temperature, and faster response and recovery times to NO gas than pure ZnO NWs. At 180 ^{o}C, In-ZnO NWs exhibited a response of 3.7 towards 8 ppm of NO with response and recovery times of 60 and 370 s, respectively.

c0012

Nanocrystalline $Na_{0.5}Fe_{2.5}O_4$: A Study of Optical, Magnetic, and Impedance Spectroscopy

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The self-propagating combustion process was applied to produce $Na_{0\cdot5}Fe_{2\cdot5}O_4$ nanoparticles, with citric acid being used as the fuel. Analysis of the XRD data indicated the production of a cubic spinel monophase with the space group ($P4_332$) and a nanometric crystallite size. According to the optical analysis, this sample shows substantial absorption in the visible region making it a promising option for optoelectronic and photovoltaic applications. Complex impedance spectroscopy was carried out in the temperature range 383 to 523 K with the frequency changing between 50 Hz and 10 MHz. The frequency dependency of the modulus was explained in the material, whereas its temperature dependence shows dielectric relaxation behaviour. The scaling law exhibits a perfect superposition of modulus spectrum in the temperature range tested which confirms that the rise of temperature does not bring any modification on the process of relaxation. In addition, the dependence of the magnetisation on the applied magnetic field has been examined.

c0014

Synthesis and Characterisation of $CdWO_4$ Nanoparticles for Photocatalytic and Dielectric Applications

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Researchers have showed a great interest in synthesizing and studying various transition metal tungstates owing to their potential applications in different areas. In the present work Cadmium tungstate nanoparticles are prepared by wet chemical method. The effect of temperature on structure, size, optical and dielectric properties are studied. Monoclinic structure of the nano product is verified by X-ray diffraction analysis and calculated crystallite size is in the range 10-25 nm. As temperature increases increased crystallite size and crystallinity is observed. Various

vibrations present in the FTIR confirm the formation of $CdWO_4$ nano particles. The Morphology and composition of the $CdWO_4$ are further studied by SEM, EDX and TEM. Energy band gap found out using Tauc method are in the range 3.5-3.6 eV. Increased absorption and a decrease in bandgap with temperature is observed. Large dielectric constant is observed for the samples indicating its profuse use as a dielectric material. Under UV light irradiation, $CdWO_4$ nanoparticles show photocatalytic degradation of Methylene blue.

c0015

Graphene Nanoplatelets Reinforced Polyvinylidene Fluoride-Hexa-Fluoro Propylene Nanocomposite for Potential Electromagnetic Interference Shielding Applications

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Graphene nanoplatelets (GNPs) based polymer nanocomposites establish themselves as an essential materials for diverse applications including electromagnetic interference shielding devices. In this work, Polyvinylidene fluoride-hexa-fluoro propylene (PVDF-HFP) based nanocomposites with 10 wt% of GNPs loading were synthesized through solvent casting technique. The electromagnetic interference shielding effectiveness (EMI SE) of GNPs@PVDF-HFP nanocomposites has been investigated in the X-band (8 GHz -12 GHz) and Ku-band (12 GHz -18 GHz) frequency ranges and the obtained values are 16.25 dB and 27.16 dB, respectively. The results of this study suggest that GNPs@PVDF-HFP nanocomposite film could be a promising material for EMI shielding devices.

c0017

Influence of Electrolyte in enhancing the electrochemical performance of polyaniline-based electrodes for supercapacitor

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Abstract: In this work, PANI nanofibers have been synthesized through the oxidative polymerization method and the effect of HCl doping on their electrochemical properties has been explored. In order to investigate the morphological and structural characteristics of the nanofibers, field emission scanning electron microscopy and X-ray diffraction were used. Galvanostatic charge-discharge and cyclic voltammetry techniques were used to evaluate the electrochemical characteristics. The cyclic voltammetry (CV) and galvanostatic charge-discharge (GCD) analysis reveals that PANI doped with 1M HCl had the highest specific capacitance 238.05 F/g and 256.25 F/g, respectively, in a 6M KOH aqueous electrolyte.

c0018

Impact of Site-selective Carbon Doping in Tuning the Spectral Features of Triangular-shaped Boron Nitride Quantum Dots

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The crucial impact of site-specific carbon doping on the electronic and optical characteristics of triangular-shaped boron nitride quantum dots having armchair and zigzag terminations (ATBNQD and ZTBNQD) are explored in-depth, within the framework of density functional theory and time-dependent density functional theory. The doping of carbon at the edge of ATBNQD opens the electronic bandgap substantially as compared to its location at the centre of the quantum dot. The computed absorption profile confirm that the site-selective C-doping is more instrumental in dictating the energy of the first/highest-intensity peak in armchair/zigzag-edged triangular-shaped boron nitride quantum dots, opening up new frontiers in designing tunable futuristic devices.

c0019

Synergistic Electrochemical Performance of $MoSSe@CoMoO_4$ Composite as Advanced Supercapacitor Electrodes

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Supercapacitors are a potential way to meet the world's energy needs going forward. We have created a Mo-based dichalcogenide called molybdenum sulfoselenide (MoSSe) as a bifunctional electrode material for supercapacitors. Additionally, the electrically conducting active edge sites of MoSSe (MoSSe@$CoMoO_4$) have changed due to the integration of $CoMoO_4$ nanorods. The MoSSe@$CoMoO_4$ symmetric cell has a specific capacity of 127.75 Fg^{-1} at 1 Ag^{-1}, an energy density of 25.55 Wh kg^{-1}, and a power density of 600 W kg^{-1}, respectively. The results show how the proposed hydrothermally assisted synthesis can create high-performing energy storage devices.

c0020

Room Temperature Synthesis of Ag@Au Core-Shell Nanostructures by Controlled Transmetallation Reaction

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Aqueous synthesis of Ag@Au core- shell nanostructures at room temperature is reported using controlled transmetallation (TM) reaction between silver nanoparticles (AgNPs) and gold precursor solution ($HAuCl_4$). The TM reaction is controlled using chicken egg shell membrane (ESM). The formation of Ag@Au core- shell nanostructures via TM reaction is confirmed using UV- Vis absorbance studies. The morphology of the synthesized nanostructures determined using the Transmission Electron Microscopy (TEM).

c0021

Studying Laminates by Tailoring Number of Layers and Arrangements for EMI shielding in X-band Range

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Due to the ever-increasing complexity of the electromagnetic environment, the market for electromagnetic interference (EMI) shielding is one of the industries that is expanding at a rapid rate. Recently, there has been a focus on developing new methods that can be used to fine-tune and forecast the shielding qualities of buildings without using up all of the raw materials. Additionally, methods that are economical and short duration of time needed for optimization have been prioritized. The strategic arrangement of electromagnetic energy-trapping layers within the impedance-matching layers is found to significantly contribute to the enhancement of absorption-dominated EMI-shielding, as demonstrated by RL studies carried out by varying the order of the conducting and magnetic layers as well as the number of layers. Among the laminates, the PC/PM/PC systems showed the best performance, with a value of -34.49 dB. PVDF-based composites comprising low-cost (MWCNTs) are used to construct the laminates for testing purposes. After doing this research, we have come up with the hypothesis that it is not required to use materials that have a high manufacturing cost and need laborious fabrication processes in order to create shielding materials that are extremely effective.

c0022

Synergistic Effect of Silver Nanoparticles on Magnetic Hyperthermia of Fe_3O_4 Nanoparticles

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The relentless pursuit of effective cancer treatments has spurred considerable interest in hyperthermia for cancer as a therapeutic modality by leveraging the vulnerability of cancer cells to elevated temperatures. This study investigates the synergistic potential of Fe_3O_4 nanoparticles combined with silver nanoparticles (SNPs) for magnetic hyperthermia applications. Utilizing the superparamagnetic properties of magnetite, the research examines the heating efficiency of these nanoparticle system under an AC magnetic field. Key experimental procedures include synthesis of Fe_3O_4 nanoparticles via co-precipitation and silver nanoparticles by chemical reduction, followed by thorough characterization using X-ray diffraction, vibrating sample magnetometry and particle size analysis. Results indicate that the incorporation of silver nanoparticles significantly enhances the thermal response of Fe_3O_4 nanoparticles, achieving higher temperatures more efficiently. The study underscores the promising potential of these combination of nanoparticles in advancing magnetic hyperthermia as a viable cancer treatment strategy, highlighting their superior heating performance.

c0023

WSe_2 Incorporated PEDOT-PSS Nanocomposite: A Highly Sensitive and Selective Electrochemical Sensor

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In the present work, we have developed a highly sensitive biosensor probe based on WSe_2/PEDOT-PSS nanocomposite system towards detection of Aflatoxin B_1 (AF-B_1), which is a carcinogenic mycotoxin. Simple electrochemical polymerization technique was carried out to prepare PEDOT-PSS over ITO electrode in presence of WSe_2. Afterwards, antibody anti-AFB_1 was immobilized over the surface of the prepared electrode in presence of glutaraldehyde cross linker. Electrochemical properties after each processing step of the developed sensor were studied through CV (cyclic voltammetry) and EIS (Electrochemical Impedance Spectroscopy). Further, DPV (differential pulse voltammetry) technique was employed to monitor the interaction between antibody (anti-AFB_1) and analyte (AF-B_1). The proposed sensor yielded a sensitivity of 14.70 $\mu A ng^{-1} mL$ within a concentration range from 11.32 ng mL^{-1} to 315.62 ng mL^{-1} for AF-B_1 detection. The limit of detection of the proposed sensor was estimated to be 45.45 ng mL^{-1}.

c0024

Magnetic Properties Of $CoCr_xFe_{2-x}O_4$ Nanomaterials Synthesized By Sol-Gel Autocombustion Route Using Double Fuel (Citric Acid And Glycine) Approach

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We report the synthesis of $CoCr_xFe_{2-x}O_4$ (where x = 0.0, 0.5, 0.9) nanomaterials using citric acid-glycine assisted sol-gel autocombustion route at 450 ºC. XRD studies for $CoCr_xFe_{2-x}O_4$ results in the confirmation of cubic spinel phase with the estimation of crystallite sizes found to vary from 25.7 nm to 26.9 nm for x = 0.0 to 0.9. The lattice constants vary from 8.3548 Å to 8.3529 Å, for x varying from 0.0 to 0.9. Raman spectra show the Raman modes (T_{2g} (3), E_g (2), E_g (1), T_{2g} (2), T_{2g} (1), A_{1g} (2) and A_{1g} (1)) corresponding to the symmetric and asymmetric stretching vibrations along with symmetric bending vibrations in the structure of $CoCr_xFe_{2-x}O_4$. Coercivity (H_c), magnetization (M) and remanent magnetization (M_r) were obtained from magnetic studies (MH curves). The considerable variation in the values of saturation magnetization (M_s) (M vs H recorded at 300 K) was observed to be 65.88 emu/g, 40.01 emu/g and 23.08 emu/g (for x = 0.0, 0.5 and 0.9, respectively) whereas the variation in values of H_c was from 1995 Oe to 1208 Oe for x = 0.0 to 0.9. The high values of H_c were observed in the MH curves recorded at 5 K for $CoCr_xFe_{2-x}O_4$ materials which were 10842 Oe, 7544 Oe and 5016 Oe for x= 0.0, 0.5 and 0.9, respectively.

c0026

Silver Oxide and Cerium-Doped Silver Oxide Nanoparticles: Synthesis, Characterization, and Photocatalytic Applications

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In this study, silver oxide (Ag_2O) and cerium-doped silver oxide (Ce-Ag_2O) nanoparticles (NPs) were synthesized using the sol-gel auto-combustion method. X-ray diffraction (XRD) was utilized to study the phase structure and composition of the nanoparticles. Fourier-transform infrared (FTIR) spectroscopy was used to identify functional groups and chemical bonding. UV-visible spectroscopy was utilized to evaluate the optical properties of the synthesized materials. The optical band gap was calculated to be 1.77 and 1.37 eV for Ag_2O and Ce-Ag_2O NPs, respectively. Photocatalytic performance was tested using methylene blue (MB) dye degradation under sunlight for 120 minutes, where Ce-Ag_2O NPs exhibited a superior degradation efficiency of 77%, significantly higher than that of pure Ag_2O NPs.

c0028

Influence of Annealing Temperature on Structural, Morphological and Optical Properties of β−Ga_2O_3

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β−Ga_2O_3 nanostructures were synthesized through solid-state combustion and comprehensively characterized to examine the influence of annealing temperature on their resulting structural, morphological, and optical properties. The XRD and Raman analysis shows that with the increase in annealing temperature, the intensity of the diffraction peaks increases, accompanied by a decrease in FWHM (Full Width at Half Maximum). EDS analysis confirms that the synthesized samples contain Ga and O as the primary elements, without any impurity. The optical properties of the samples are investigated with UV-Vis DRS showed an absorption edge occurring between 236 to 242 nm. The calculated optical bandgap of the synthesized β-Ga_2O_3 nanostructures falls within the range of 4.5 to 4.6 eV.

c0029

Degradation of MB Dye by Bio-Synthesized V_2O_5

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The pure phase of V_2O_5 nanoparticles has been synthesized by the bio-synthesis route using Morus Alba leaf extract. XRD pattern confirms the orthorhombic crystal symmetry. SEM image reveals the pseudospherical morphology with an average grain size of ~ 120 nm. The Tauc plot of the reflectance spectrum estimated the direct band gap as ~ 2.27 eV. V_2O_5 nanoparticles were utilized to degrade the Methylene Blue dye under sunlight.

c0032

Biosynthesis of NiO Nanoparticles using Artocarpus heterophyllus Leaf Extract: Structural, Optical and Antioxidant studies.

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. The work aimed to explore the biosynthesised Nickel Oxide (NiO) Nano-Particles (NPs)' structural, optical properties and antioxidant efficacy using Artocarpus heterophyllus leaf extract (Ah-NiO NPs) through co-precipitation. The average crystallite size, dislocation density, and micro-strain were evaluated using the Debye-Scherrer, Size-Strain Plot (SSP), and Halder-Wagner (H-W) method using XRD results. The absorption peak of Ah- NiO NPs was noticed at 312.31 nm in the UV region. The optical conductivity spectrum demonstrates the prepared Ah-NiO NPs might have a direct band gap. FTIR spectrum shows the stretching vibrations of Ni-O at the wavenumber 555 cm^{-1}. The EDAX spectrum shows the elemental composition in the weight percentages of Ni (67.25%), O (24.05%) and C (8.70%). XRD, UV-visible, FTIR and EDAX results confirmed the formation of Ah-NiO nanoparticles. The antioxidant activity of Ah-NiO NPs was examined using the DPPH method. The biosynthesised Ah-NiO NPs could have potent applications in optoelectronics and pharmaceutical fields.

c0033

Site-Selective Photoluminescence and Multi-Color Emission via Vis/NIR Dual Mode Excitation of Rare-Earth Doped Inorganic Nanophosphors

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Numerous possibilities open in the domain of nanophosphors when excitation is shifted from 980 nm to multiple excitation wavelengths. Multi chromaticity can be obtained by variation in chemical composition, phase, and structure, but command over the color spectrum from a fixed composition is challenging. Here, we present a practicable and adaptable method for achieving modulated luminescence and site selectivity throughout the visible spectrum through dual-mode excitation. A series of photostable, cubic $KLaF_4$: Er^{3+}/Yb^{3+}/Eu^{3+} nanoparticles bearing a size of nearly 9 nm have been synthesized through the wet chemical method. Powder X-ray diffraction and High-Resolution Transmission Electron Microscopy reflect on the nanoparticles' crystallinity and nano-size distribution. Spatial

photoluminescence mapping substantiates the homogeneity of doping and applicability of the nanoparticles. Thus, by utilizing the intense dual-wavelength photoluminescence signal, this work can be expanded to explore similar effects in other rare earth-doped systems pumped by multiple-wavelength lasers and introduces fresh opportunities for applications such as upconversion color displays, white light generation, super-resolution microscopy, and bioimaging.

c0035

AuNPs@Ag Nanodendrites for Volatile Organic Compound Detection based on Surface Enhanced Raman Scattering

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We demonstrate the fabrication and application of AuNPs decorated AgNDs for SERS-based detection of volatile organic compounds (VOC) such as acetone and ethanol. A facile electroless deposition approach has been adopted to make symmetric AgNDs with high-density hot spots. The stability and sensing capabilities were enthused to the next level by incorporating AuNPs over the AgNDs surface. The characteristic signatures of acetone and ethanol vapor at 776 cm-1 and 842 cm-1, respectively, are observed in the surface-enhanced Raman signals. The trace-level detection of acetone and ethanol vapor is important for diagnosing diabetes.

c0036

Lead and Rare Earth-Free Cesium Based Inorganic Metal Halide Perovskite Material for High Luminescence Bright White Light Emission

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Metal halide perovskites have emerged as promising materials for optoelectronic devices, including Light Emitting Diodes (LEDs). However, achieving high photoluminescence quantum yield (PLQY) remains a challenge. This paper presents the synthesis and characterization of an eco-friendly, low-cost, and stable lead and rare earth-free $Cs_3[Bi_x - In_{1-x}]_2Br_9$ perovskite material for White Light LEDs (WLEDs) under UV excitation. The perovskite was synthesized using a solvothermal method, and its crystal structure and phase were analyzed through X-ray diffraction (XRD). Scanning Electron Microscopy (SEM) and Energy Dispersive X-ray spectroscopy (EDX) confirmed the morphology and composition of the material. Transmission Electron Microscopy (TEM) revealed the formation of nanocrystals (NCs) with good crystal orientation. UV-Vis absorption and photoluminescence (PL) spectroscopies were employed to investigate the optical properties, demonstrating bluish-white light emission after introducing Indium (In) at 0.3% and 0.5% weight percentages. The perovskite showed potential for efficient, cost-effective WLEDs, highlighting its significance for advancing perovskite-based LED technology.

c0037

TiO_2 Nanotubes and rGO Nanocomposite Integrated Electrochemical Sensor for Cd^{2+} Ion Detection

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The nanocomposite of TiO_2 nano tubes and reduced graphene oxide was successfully synthesised via alkaline hydrothermal method. The structural and morphological properties of the composite were determined by XRD, Raman, and SEM characterizations. In this work, the composite was explored as an electrochemical sensor for the detection of cadmium ions in water. Cyclic voltammetry (CV) was employed to study the electrochemical properties of the composite, and differential pulse anodic stripping voltammetry (DPASV) analysis was employed to investigate the quantitative detection of Cd^{2+}ions under optimal conditions. The nanocomposite exhibited enhanced voltametric responses in detection of Cd^{2+} ions, compared to its individual components.

c0039

Tunning of Structural and Magnetic Properties of $MnFe_2O_4$ Nanoparticles Through Cerium Ion Substitution

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Present investigation reports the impact of Ce doping on structural and magnetic properties of $MnFe_2O_4$ NPs. The NPs were successfully synthesized through citric acid assisted sol gel auto-combustion method. The synthesized NPs were characterized through X-ray diffractometer (XRD), Fourier transform infrared (FTIR) spectroscopy and vibrating sample magnetometer (VSM) to investigate structural, chemical and magnetic properties. All pristine as well as Ce doped NPs were found in pure spinel phase with Fd3m space group. Crystallite size and lattice parameter were found in the range of 9±1 to 19.4±0.3nm and 8.366±0.007 to 8.395±0.0003 Å, respectively. FTIR spectra showed the presence of characteristic bands correspond to tetrahedral and octahedral lattice vibrations. All magnetic characteristics were found to be decreased with addition of Ce ion which was further decreased with increase in concentration of Ce ions. Saturation magnetization was observed to be decreased from 49 emu/g ($MnFe_2O_4$) to 12 emu/g (for $MnCe_{0.15}Fe_{1.85}O_4$). Similarly, remanence magnetization was found to be decreased from 19 emu/g ($MnFe_2O_4$) to 12 emu/g (for $MnCe_{0.15}Fe_{1.85}O_4$). The variations were resulted through larger ionic radii and lower magnetic moment of Ce in comparison to Fe. Therefore, it is concluded that the Ce ion substitutions have significant effect on structural and magnetic properties of $MnFe_2O_4$ NPs. So, Ce ion doping could be useful for the fine tuning of characteristics of $MnFe_2O_4$ NPs and can be used for material engineering as per requirement of specific application.

c0040

An Electrospinning Approach Towards The Production of Bio Degradable Mulch Films

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A true revolution in agriculture was brought about by the invention of plastic technology. Mulch films are one of plastics that have been utilised to enhance crop protection and yields. They are helpful in raising soil and air temperatures, shielding plants from various threats, enhancing water management, inhibiting the growth of weeds, and, ultimately, preventing an excessive reliance on agrochems. The synthetic polymers from non-renewable resources has been utilised because of its low cost, easy processing, resistance to all forms of degradation, and mechanical and barrier qualities. But, because of its poor biodegradability, during disposal it adversely affect on the ecology and economy. The introduction of biodegradable mulch films mainly the starch-based bio-composite mulch films helps to replace conventional mulch films, able to resolve the issues mentioned are interpreted in this paper.

c0041

Exploring The Structural and Optical Properties of La^{3+} Doped $MnWO_4$ Nanostructures

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To synthesize $La_xMn_{1-x}WO_4$ nanomaterial (where x= 0.0, 0.01, 0.03, and 0.05), a precursor obtained through the co-precipitation method and sintered at different temperatures but the best crystallinity was found at 800°C. Lanthanum (La^{3+}) was added during the preparation of the precursor to improve the performance of structural and optical properties of crystalline $MnWO_4$ under optimal sintering temperature conditions. Consequently, it was proposed that the degradation of organics such as methylene blue (MB) is more efficient when tert-butyl hydrogen peroxide(TBHP) is used as the oxidizing agent in water at ambient temperature, facilitated by the incorporation of La^{3+} ions in $MnWO_4$ system and we observed that 1% La-doped sample shows a significant reduction in the energy bandgap value as compared to pure sample.

c0042

Influence of Gd-Cu co-doping on the Structural and Morphological Properties of Cobalt Oxide

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In the present work, nanoparticles of pristine and Gd and Cu co-doped cobalt oxide with chemical formula $Co_{3-(x+y)}Cu_xGd_yO_4$ (x=0.0,0.05,0.1,0.2 and y=0.1) have been synthesized via co-precipitation method. X-ray diffraction reveals the desired phase formation and crystal symmetry of the synthesized samples. The crystallite sizes are

calculated using the Debye-Sherrer equation and Williamson-Hall method and are found to decrease with the increase in doping. FTIR and Raman spectra confirm the presence of characteristic vibrational bands and thus successful formation of spinel structure of cobalt oxide. Morphology of the samples is studied using FESEM micrographs along with the EDAX spectra. The determined grain sizes are found to decrease with the doping.

c0047

Water Desalination Using Graphyne Membranes: MD Simulation Approach

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This study reports the use of γ-graphyne and graphyne-2 (also known as graphdiyne) as a porous membrane for water desalination using molecular dynamics (MD) simulations. The Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) was utilized to simulate the equilibrium state of the membrane and added salt ions (Na+ and Cl-) with added water molecules with salinity equal to seawater. Lennard-Jones (LJ) potential was applied to explain non-bonded interactions between the membrane and ions and water molecules, in terms of energy values. The snapshots were taken from the evolution of the desalination phenomenon. The molecular patterns of accumulation of ions in the vicinity of the membrane were also captured as functions of the energies of the interaction between the contaminants and porous membrane. The ion rejection ratio, mean square displacement (MSD), and ion diffusivity were calculated along with the radial distribution function (RDF), indicating the dynamics of the separation process.

c0048

Influence of Cu substitution on the Structural and Optical Properties of $SmFeO_3$ Nanomaterials

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This work elucidates the effect of Cu substitution on the structural and optical properties of $SmFeO_3$ nanocrystalline samples synthesized via sol-gel citrate route. Rietveld refinement of X-ray diffraction (XRD)patterns reveals phase purity and orthorhombic crystal symmetry (Pbnm space-group) of the samples. Crystallite sizes lie in the range 48-57 nm while lattice strain is of the order of 10^{-3} evaluated using Williamson Hall analysis. Cu substitution causes the increase in the crystallite size, lattice strain, bond-length and bond-angle while shrinkage in the unit cell volume. Fourier-transform infrared spectroscopy (FTIR) confirms two active vibrational bands corresponding to Fe-O and O-Fe-O band, this further validates the successful formation of the typical perovskite structure. The shifting in the absorption bands towards higher wavenumber with Cu doping is concomitant with the x-ray diffraction results. The optical energy band gap exhibits redshift in the Cu doped sample, this might be due the creation of oxygen vacancies and generation of extra energy states near the conduction band.

c0050

Temperature Dependent Tunable Optical Property Analysis of In_2Se_3 Thin Films

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In this research work, we performed the systematic analysis of the effect of annealing temperature and annealing time period on the optical properties of In_2Se_3 films deposited on glass slide by using thermal vapor deposition setup. In general, the deposited films at room temperature are amorphous in nature. Here in this part of research our aim to estimate the nature of variation of optical band gap of 30 nm thin film of In_2Se_3 by varying the annealing temperature and annealing time period. To evaluate the band gap of heat-treated In_2Se_3 samples; we did the UV-visible absorption spectra analysis of these films and we find out that the optical band gap of In_2Se_3 films increases as we increase the heating temperatures and heating time period. The effects of heating temperatures and heating time period are more prominent when we treating films at temperature higher than 100 °C and for a time period of more than 5 min. The observed band gap turnability of In_2Se_3 by varying different heating parameters shows that it can be useful for various application purposes.

c0051

Enhanced Electrochemical Performance of Cr-doped MoS_2/$CuCo_2S_4$ Binary Composite for Supercapacitors

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The synergistic effect of transition metal doping and composite formation can be imperative to improve the limited conductivity and inferior cyclic stability of MoS_2 for supercapacitors. In this work, the binary composite of Cr-doped MoS_2 (CrMS-5) with $CuCo_2S_4$ (CCS) is synthesized via hydrothermal method. The CrMS-5/CCS composite delivered tremendous capacitance of 1324.08 F g^{-1} at 4 A g^{-1}. The outstanding performance of doped composite is due to synergism between doping and composite formation Furthermore, the device attained a high energy (183.9 Wh kg^{-1}) and power density (4 kW kg^{-1}), along with high cyclic stability of 81% for 5,000 cycles. The device illuminated a star-shaped LED panel of 12 red LEDs for 30 minutes. Thus, the results demonstrate the superiority of doped MoS_2-based composites for high-energy supercapacitors.

c0052

A Study of Structure and Morphological Properties of NiO and NiO@GO nanocomposites

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Nanocrystalline samples of NiO and NiO@GO have been successfully synthesized using sol-gel auto combustion route and simple sonication technique respectively. The structural and morphological properties of synthesized samples are examined. X-ray diffraction (XRD) patterns reveal that the samples have been successfully formed in the standard cubic phase of NiO and traces of GO is found in the nanocomposite. The SEM micrographs depict the irregular spherical shape of particles and EDS spectra reveals the presence of constituent elements on the surface of synthesized nano samples. Using imageJ software, the nominal particle size from SEM images and average crystallite size using Debye-Scherrer formula are calculated and reduction in both cases have been observed due to the presence of GO sheet incorporated with NiO nanoparticles.

c0053

Molecular Dynamics Simulation Study for the Mechanical Properties of SWCNT/PVA Composite with Stone-Wales Defects

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The extraordinary mechanical properties of carbon nanotubes (CNTs) have drawn special attention from composite scientists to prepare super strong composite materials for various applications. However, the degrading factors like defects inside the CNTs are sometimes play crucial role in finding the exact strength or stiffness of their composites. These defects are created inevitably during the manufacturing process or in the purification procedure. In this work, the mechanical properties of a single walled carbon nanotube/polyvinyl alcohol composite with a constant volume fraction are simulated with varying number of Stone-Wales (SW) defects inside the CNT structure. The positions of the defects are also changed and the mechanical properties of the composite are calculated by Molecular Dynamics simulation. Significant changes in the mechanical properties are observed in some defect positions, clearly stating about the dependence of their mechanical response on the SW defects including their number and pattern of distribution inside the CNT structure.

c0054

Pressureless Sintering of Ti_3AlC_2 and Cr_2TiAlC_2 MAX phases

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MAX phases are ternary layered transition metal carbides and nitrates which has immense applications in high temperature protective coatings. MAX are the parent precursors for synthesizing conductive 2-dimensional MXene inks. Here, the MAX phases of Ti_3AlC_2 and Cr_2TiAlC_2 are synthesized by mixing the elemental precursors at an

appropriate stochiometric ratio via a high energy milling and sintered them at high temperatures 1500˚C and 1600˚C respectively under inert atmosphere for 2 hrs. The structural analysis of the pristine MAX phases is confirmed through XRD analysis. It is observed that relatively low-ball milling time of 10 hrs produce a phase pure Ti_3AlC_2 and Cr_2TiAlC_2 MAX phase.

c0055

Highly Stable and Luminescent Formamidinium Based Perovskite Nanocrystals' Probe for Temperature and Mercury Sensors and In-vitro Imaging in Living Cells.

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Now a days lead halide perovskite ($APbX_3$: X=Cl, Br, I) nanocrystals (NCs) have engrossed massive devotion to researchers because of their fascinating photophysical properties which make them suitable for various optoelectronic, sensing, and bioimaging applications. However, the current issues with MA and Cs based compounds that they chemically decompose quickly at elevated temperature and intense light. The perovskite phase also degrades rapidly due to the ionic nature and the presence of dynamic organic capping ligands around the NCs. Comparatively better light and thermal stabilities of formamidnium lead halide ($FAPbX_3$) materials and limited reports encourage us to further explore their inherent properties. Herein, we report a facile synthesis method of Cs-doped $FAPbBr_3$ NCs by facile ligand-assisted reprecipitation (LARP) synthesis approach. To improve the structural stability, we encapsulated different shelling materials such as polymethylmethacrylate (PMMA), SiO_2, and double-coated SiO_2-PMMA around the NCs. The double-coated NCs exhibit superior heat and water stabilities, and retain their emission intensity over a month while dipped in DI water. The film was also tested as a temperature sensor that revealed quite good sensitivites. We executed these stable double-coated NCs as a fluorescent probe for the detection of highly toxic Hg^{2+}-ions and cell imaging, which are advantageous for both cost-effective sensing and bio-imaging applications.

c0056

Cross-sectional Transmission Electron Microscopy Study of As-grown CuO nanowire Sample Synthesized by Thermal Oxidation Method

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Cross-sectional Transmission Electron Microscope (XTEM) investigation of as-grown CuO nanowires sample, synthesized by thermal oxidation method, has been carried out to find out the origin of the growth mechanism that may be present in the underlying oxide layers on which the nanowires grow. The TEM measurement invariably showed the presence of twin bands almost everywhere in the CuO layer and the nanowires grow at the junction of these twin bands. The as-grown samples were also analyzed by the Scanning Electron Microscope (SEM).

c0058

Synthesis of Zinc Nano Powder by Electrical Explosion of Wire Method

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The synthesis of Zinc Nano powder through electrical explosion of wire (EEW) is a novel and efficient method to produce high-purity, ultrafine Zinc particles. In this process, a Zinc wire is subjected to a high-voltage electrical pulse, causing rapid heating, melting, and vaporization of the wire material. The subsequent rapid cooling and condensation of the vapor result in the formation of zinc Nano powder. Zinc and Zinc oxide Nano powder has wide range of industrial applications. Their inherent antimicrobial property, nontoxic nature and lesser cost than silver, make them suitable for medical industry. Bulk production of Zinc and Zinc oxide Nano powder is possible by Exploding wire technique which is top down physical method to produce metal and its alloy Nano powder.

c0062

Luminescence Effects of Carbon Dot Decoration on SnSe Nanosheets

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Group IV-VI metal monochalcogenides (MMCs) are a class of anisotropic, layered materials with orthorhombic crystal structure and 1:1 stoichiometry. Tin selenide (SnSe) is a particularly notable MMC due to its high chemical and thermodynamic stability, tunable band gap, and exceptional optical absorption. In this study, we developed a hybrid nanosystem by decorating SnSe nanosheets with carbon dots (C-Dots). Bulk SnSe was exfoliated via liquid phase exfoliation (LPE) to obtain nanosheets, and water-soluble C-Dots were synthesized using a one-step microwave method. The SnSe/C-Dot hybrid was then synthesized through a hydrothermal approach. Raman spectroscopy revealed a few characteristic SnSe peaks and two distinct peaks at 1361.2 cm^{-1} and 1574.2 cm^{-1} which belong to the D and G bands of carbon, indicating the incorporation of C-Dots. Elemental mapping demonstrated a uniform distribution of C-Dots on the SnSe nanosheets. Notably, SnSe on its own displayed a unique excitation wavelength-dependent photoluminescence (PL) feature. PL spectroscopy also showed a ~9.6% increase in the emission peak intensity for the SnSe/C-Dot nanohybrid compared to its SnSe counterpart.

c0063

Investigation of the effect of gamma irradiation on the structural and magnetic properties of Ni-Co ferrite/ graphene oxide nanocomposite

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Present work reports structural and magnetic studies of $Ni_{0.5}Co_{0.5}Fe_2O_4$/graphene oxide (NCF/GO) nanocomposite irradiated with different doses (25 and 50 kGy) of ^{60}Co gamma radiation. The structural and magnetic properties of all the samples were investigated by powder X-ray diffraction (XRD), Fourier transform infrared (FT-IR) and vibrating sample magnetometer (VSM). The crystallite size was found in the range of 22 - 42 nm. The crystallite size was increased after gamma irradiation and was found to be increasing with increase in dose of gamma radiation. FTIR spectra of NCF/GO nanocomposite showed the presence of absorption bands correspond to both NCF and GO, which confirmed the successful formation of nanocomposite. The peak intensity of absorption bands in FTIR spectra was found to be reduced after gamma irradiation, which was father reduced with increase in dose. The saturation magnetization and coercivity were found in the range of 57-48 emu/g and 787-776 Oe, respectively. The saturation magnetization and coercivity were decreased after gamma irradiation.

c0065

Effect of Nd Doping on the Structural, Morphological and Magnetic Properties of Strontium Hexaferrite Nanoparticles

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In this work, we conducted a study to investigate the impact of Nd doping on the structural, morphological, and magnetic characteristics of M-type strontium hexaferrite $Sr_{1-x}Nd_xFe_{12}O_{19}$ ($0 \leq x \leq 0.50$) nanoparticles. The nanoparticles were synthesized using co-precipitation method. The XRD analysis demonstrated the purity of the samples and crystallite size ranging from 35 to 55 nm. The structural confirmation of the samples was achieved through Raman and FTIR spectroscopy, which revealed characteristic peaks at specific wavenumbers corresponding to the expected crystal structures. Morphological studies conducted using FESEM exhibited a change of particles shape from hexahedral to flaky shapes as a result of doping. EDAX spectra showed no presence of impurity elements in the samples. The M-H loops depicted a reduction in saturation magnetization from 43 to 21 emu/g for the higher Nd doped sample. Moreover, coercive field and remanence magnetization were found to decrease with increasing doping levels.

c0066

Antibacterial And Photocatalytic Activities Of G-C3N4/STO For Biomedical And Water Treatment Application

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Here the production of Graphitic carbon nitride (g-C3N4) and its doping with strontium titanate nanopowder (SrTiO3) (STO), as well as the methodical investigation of photocatalytic dye degradation of Rhodamine B (RhB) dye, have been investigated. Both the morphological and structural analyses verified that the produced materials had formed correctly. its antibacterial characteristics were examined using the Muller-Hinton technique. At last Excellent degradation efficiencies over a 0-60 minute period were achieved by the photocatalytic degradation of g-C3N4/STO by breaking down Rhodamine B under UV light. According to these findings, g-C3N4/STO is appropriate for industrial applications including biological and water treatment.

c0067

Reduced Graphene Oxide Using Graphene by Modified Hummer Process

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From last two decades Graphene(G) related materials attracted more attention of researchers due to their non presidential properties and applications. Various preparation methods have been employed for the preparation of Graphene related materials. In this paper reduced graphene (r-GO) was prepared by modified Hummer's method using graphene as a starting material. The temperature of annealing was optimized to obtain reduced graphene oxide. The graphene and prepared Graphene oxide (GO)/Reduced Graphene oxide (r-GO) were characterized by X-ray diffraction and Raman Spectroscopy.

c0068

Increased Defect Sites and Enhanced Fluoride Adsorption by Nanocomposite of Silver Oxide and Hydrogen Tri Titanate Nanotubes

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A nanocomposite of hydrogen tri titanate nanotube and silver oxide was developed using a twostep simple synthesis route. The composite formation was confirmed through XRD and TEM characterizations. Further optical properties of the nanocomposite were studied using the UV-Visible spectroscopy. The data was further utilised to calculate the Urbach energy. The increased Urbach energy of the composite indicated a higher number of defect sites which further contributed to enhanced absorption properties. Further the nanocomposite was explored for adsorption of fluoride from water. The fluoride adsorption capacity of the nanocomposite was found to be 165 mg/g which is 3 times higher than that of hydrogen tri titanate nanotubes.

c0069

Heterostructured Nanocomposite of $MgFe_2O_4/MoO_3$ for Detection of H_2S

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A heterostructured nanocomposite of magnesium ferrite ($MgFe_2O_4$) and molybdenum trioxide (MoO_3) was synthesized for the detection of hydrogen sulfide (H_2S). The crystalline structure and elemental composition of the material were examined through X-ray diffraction and X-ray photoelectron spectroscopy. Field emission scanning electron microscopy confirmed the nanosheet structure of MoO_3 and nanoparticles of $MgFe_2O_4$. The decrease in the

band gap of the composite material is confirmed through UV-visible Spectroscopy, and the surface area of the materials was measured by Brunauer-Emmett-Teller. An enhanced H_2S sensing performance was noted in MM2 nanocomposite (20 % MoO_3) which possesses a 1.86 time greater response to H_2S than pure $MgFe_2O_4$ at 135 °C. The response of the MM2 composite was 31.18 % for 7 ppm concentration at 135 °C.

c0071

Exploring the Electronic and Optical Properties of Armchair SiC (8,8) SWNTs Using First-Principles Calculations

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Single-walled silicon carbide (SiC) nanotubes have garnered significant interest due to their unique properties and potential applications in optoelectronic devices, light-emitting diodes (LEDs), energy storage materials, and photovoltaic systems. In this study, density functional theory (DFT) combined with the universal force field method was employed to investigate the electronic and optical properties of armchair (8,8) SiC nanotubes through first-principles calculations. The simulation results indicate that the armchair (8,8) SiCNT exhibits characteristics of an indirect band gap semiconductor. The optical properties, including absorption spectra, reflectivity, conductivity, and refractive index, were characterized across various spectral regions.

c0073

Dimensions in Focus: Investigating the Impact of Lateral Size on the Electrical Properties of $Ti_3C_2T_x$ MXene

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In this study, we explore the impact of the lateral size of MXene on its electrical properties. We developed $Ti_3C_2T_x$ MXene sheets using a chemical etching route. Many properties and applications of the MXene depend on its flake size. In this study, we developed three different lateral sizes of $Ti_3C_2T_x$ MXene material and investigated how and why the electrical conductivity changes as the lateral size of the MXene varies. The electrical conductivity of the larger flake MXene sample (~730 S/m) is four times that of the smaller flake size samples.

c0077

Degradation studies of Dichlorvos Pesticides using Copper Nanoparticles

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In this study, stable suspension of copper nanoparticles (CuNPs) was prepared by adding a specific amount of isopropanol solvent and surfactant i.e. oleic acid. X-ray diffraction (XRD) was used to estimate particle size and phase analysis of Cu nanopowder. Prepared Cu nanosuspension was characterized by UV-Vis and Fourier Transform Infrared (FTIR) spectroscopy. UV Vis data after 60 days showed a very broad UV-Vis peak obtained in the 243-261 nm with maximum absorbance at around 249 nm with a very weak absorbance in 325-380 nm range, which signs the stability of Cu nanosuspension. To investigate the disintegration of pesticides, solutions of different concentrations of dichlorvos (DDVP) pesticide were prepared. A specific amount of Cu nanosuspension was added to prepared pesticide solutions and the color change of the samples was observed with time. UV- Vis and FTIR spectroscopy were used to characterize the reaction products. The redshift in UV-Vis Plasmon of nanosuspension added in DDVP solution inferred the degradation of DDVP. The FTIR spectra show that the peaks observed at 1150 cm^{-1} and 870 cm^{-1}, due to P=O and C–O vibrational bonds respectively, present in DDVP, were absent in the reaction samples. This confirms the degradation of the organic bonds of dichlorvos.

c0078

Phonon Confinement and Size Effect in the Raman Modes of $K_{0.5}Na_{0.5}NbO_3$ Lead-free Ceramics

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To investigate the relationship between the grain size and the Raman modes of lead-free ceramics $K_{0.5}Na_{0.5}NbO_3$ (KNN), a comprehensive study on the impact of different synthesis techniques on Raman spectroscopy is presented. Conventional solid-state method and hydrothermal method are used to prepare the KNN ceramics to obtain different grain sizes. The phonon confinement effect (PCE) explains the grain size effect on the changes in the Raman spectra. Asymmetric broadening and intensity variation observed in Raman peaks of KNN samples is corelated with grain size and PCE. To illustrate the agreement between the predictions of experimental Raman data and PCE, the present study incorporates effects such as grain and crystallite size distribution. The computed Raman spectrum obtained from density functional theory (DFT) is found to agree well with the experimental spectrum.

c0079

Structural and optical properties of zinc oxide nanoparticles for Rhodamine B dye degradation under visible light

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This research communication focuses on synthesis of zinc oxide (ZnO) nanoparticles and their characterization by X-ray diffraction (XRD), FTIR, and UV-visible spectroscopy technique. The X-ray analysis confirm the single-phase wurtzite structure with space group $P6_3mc$. The values of lattice constant, crystallite size, lattice strain were calculated using standard relation. The ZnO nanoparticles were also characterized by FTIR spectra which reveals the presence of various functional group such as O-H. The optical band gap of the order of 3.04 eV was obtained through UV-Visible spectroscopy. The dye degradation of Rhodamine B was performed using ZnO nanoparticles which suggests the efficiency of dye degradation as 80%.

c0080

Cobalt Ferrite Magnetic Nanoparticles as Highly Efficient, Recoverable Nanocatalyst for Photocatalytic Application

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A highly efficient, recoverable and reusable magnetic nanocatalyst cobalt ferrite (CoFe2O4) was prepared by low temperature sol-gel auto-combustion method. XRD, FE-SEM, FTIR, VSM and UV-Visible techniques were employed to characterize the prepared cobalt ferrite nanoparticles. Single phase cubic spinel structure was observed through XRD analysis. Two main absorption bands are observed in FTIR spectrum. VSM study indicates the enhancement in the saturation magnetization of the order of 77.8 emu/g. The optical band gap of the order of 1.83 eV was obtained through UV-Visible data showing semiconducting behavior useful for photocatalytic applications. MB dye was degraded by CoFe2O4 nanoparticles giving efficiency of 90%.

c0081

Enhanced Photocatalytic Activity of Pd/MoS_2 based Nanocomposites for Degradation of Organic Pollutants and Antibiotic Tetracycline

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Herein, Pd/MoS_2 nanocomposites were successfully synthesized to evaluate their photocatalytic performance for degradation of organic pollutants and antibiotics under simulated solar light irradiation. The Pd-decorated MoS_2 unveiled exceptional photocatalytic activity for degradation of 98 % of Rhodamine (RhB) and methylene blue (MB), 96 % of tetracycline (TC) with in short interval of time as compared to bare MoS_2. The enhanced photocatalytic performance can be attributed to the incorporation of Pd, which improves light absorption, increases the specific surface area, and reduces the recombination of photoinduced charge carriers. These factors collectively facilitate a significant increase in overall photocatalytic activity.

c0082

Mixed State of rGO/GO for Efficient Removal of Cadmium Ion from Water

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The green and facile approach to synthesize a two dimensional nano-hybrid of reduced graphene oxide(rGO) /graphene oxide (GO) was successfully achieved. The material characterization confirmed the mixed state of rGO/GO. The preparation using inexpensive source – sugar, from local markets and the high yield along with a very short synthesis time makes it possible to scale up the procedure. Further, the developed material was employed in removal of hazardous contaminant, cadmium, from water. It was possible to achieve 70 % of Cd^{2+} removal from 1 L of water with the use of 1g of the material. The production cost of 1g of material is as low as 20 paise, making the method highly cost effective. Therefore, this work reports an economic and efficient material for removal of toxic contaminant, cadmium ion, from water, serving as a pathway to develop nanomaterial based filters for removal of cadmium.

c0083

Synthesis of polymer functionalized manganese iron oxide nanoparticles by using thermal decomposition method in magnetically activated hyperthermia therapy

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Magnetic hyperthermia, utilizing magnetic nanoparticles (MNPs), shows significant potential as an adjunct cancer treatment due to MNPs ability to generate heat when exposed to an alternating magnetic field (AMF). In this study, manganese iron oxide nanoparticles were synthesized via the thermal decomposition method. The resulting nanoparticles, confirmed to have a cubic spinel structure through X-ray diffraction, transmission electron microscopy, Fourier transform infrared spectroscopy, and vibrating sample magnetometry, were monodisperse with an average size of 22.75 ± 0.17 nm and excellent cubic morphology. The specific absorption rate (SAR) and intrinsic loss power of the nanoparticles were 154.67 W/g at a clinical field maximum of 352.2 Oe and a frequency of 277 kHz. After m-PEG functionalization, the SAR increased to 342.08 W/g at the same field. These results highlight the potential of enhanced magnetic heating efficiency of functionalized manganese iron oxide nanoparticles, suggesting promising advancements in hyperthermia as an alternative cancer therapy.

c0084

Development of assembly of Iron Oxide nanoflakes for magnetic properties study and application as T1 MRI contrast agent

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The magnetic properties of the 2D iron oxide nanoflakes have been explored by synthesizing an assembly structure of the nanoparticles. The developed system shows hysteresis nature at very low temperatures as well, where the coercivity and remanence values have been seen to decrease with increasing temperatures. The thermo-magnetic studies reveal the existence of magnetic frustration in the system which is evident from the splitting in the M_{ZFC} and M_{FC} curves at low temperatures. The developed system is also showing a positive response as a possible T_1 MRI contrast agent after an increasing trend in the longitudinal relaxation rate and the value of r_2/r_1 less than 10 has been observed.

c0085

Fowler Formula for Photoionization Spectra of Small Lanthanum Clusters

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Abstract : In this study, we show that the traditional Fowler theory of surface photoemission effectively fits the photoabsorption profile shapes of neutral La_n clusters(n=2-10). The internal cluster temperatures match well with those expected for a collection of freely evaporating clusters. Building on previous work with indium clusters, these findings suggest that the straightforward and physical Fowler model could be highly useful in metal-cluster spectroscopy. We also hope these results will stimulate a thorough theoretical examination of how bulk-derived models apply to cluster photoionization and the shift from atomic and molecular to surface-type photoemission.

c0088

SnO_2 nanoflower-based formaldehyde sensor for recognizing food adulteration

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In this work, a chemiresistor was developed to detect formaldehyde vapors using SnO_2 nanostructure. The sensing material was synthesized by use of a low-temperature hydrothermal process. The synthesized material was characterized using the field emission scanning electron microscope (FESEM) and X-ray diffraction (XRD) techniques. The sensing material was meticulously drop-cast over electrodes that were interdigitated with gold to fabricate the sensor device. Using a customized gas test apparatus, the sensing performance was examined. The sensor exhibited higher sensitivity towards formaldehyde. In the presence of 100 ppm formaldehyde, a response of 25 was observed. The sensor's theoretical limit of detection is 1 ppm. The proposed sensor is appropriate for monitoring formaldehyde vapors emitted from adulterated food.

c0089

Hydrothermally Synthesized Titanium Dioxide Nanorods Assembled in Rice Ball Morphology for Application in Ultraviolet Light Detection.

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Titanium dioxide nanorods were synthesized by a single step hydrothermal process using titanium butoxide precursor. Field emission scanning electron microscopy showed that the nanorods were self-assembled to form porous microspheres resembling rice balls. The nanorods crystalized in tetragonal rutile structure according to X-ray diffraction analysis. The average crystallite size for the synthesized TiO2 nanoparticles range from 4-18 nm. The optical properties of nanorods were studied by diffuse reflectance spectroscopy and their bandgaps were estimated using Tauc's plots. Ultraviolet light sensing activities were studied by illuminating the doctor bladed TiO_2 nanorod films with a 16 W, 312 nm UV lamp. The results indicate that our TiO_2 nanorods have potential application in the field of ultraviolet light detectors.

c0090

Enhanced Room Temperature Ammonia Gas Sensing in La Doped ZnO Nanorods

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The detection of ammonia is critical for industrial safety and clinical diagnostics due to its adverse health effects even at low concentrations. Heater-free detection of ammonia at room temperature is essential for sensor miniaturization and energy conservation. We have fabricated room temperature Zinc Oxide(ZnO) nanorods based ammonia gas sensor and enhanced its performance using Lanthanum(La) doping. Indium Tin Oxide (ITO) inter-digitated electrodes (IDE) were fabricated on glass substrates via UV photolithography. A ZnO seed layer (200 ± 5 nm thick) was deposited on the ITO-IDE at room temperature using RF magnetron sputtering with an $Ar:O_2$ ratio of 5:3. ZnO nanorods were synthesized on ZnO-seeded ITO IDE substrates using hexamethylenetetramine and zinc nitrate hexahydrate as precursors. 0.5% La doping was achieved by incorporating lanthanum chloride heptahydrate into the ZnO nanorods via hydrothermal growth process conducted at 95 °C. Structural characterizations using x-ray diffraction shows a

strong peak at 34.8° which shows a c-axis oriented growth of ZnO in hexagonal wurtzite phase and morphological characterization using field emission scanning electron microscopy (FESEM) confirmed the presence of vertically aligned ZnO nanorods. Exposure to 250 ppm ammonia gas decreased resistance of ZnO nanorods based sensor from ~ 0.19 MΩ to ~ 59 kΩ while the resistance of the 0.5 % La doped ZnO nanorods from ~ 4.6 kΩ to ~ 0.89 kΩ. The 0.5 % La doped ZnO nanorods based sensor exhibited a faster response time of ~ 13 s, and an enhanced responsivity of ~ 85 %. The low-cost, biocompatible, and compact ZnO-based ammonia gas sensors with high responsivity demonstrate immense potential for room temperature ammonia sensing applications.

c0091

Exploring Gold Nanoparticle Morphologies for Enhanced Surface-Enhanced Raman Scattering (SERS) Applications

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The impact of gold nanoparticle shape on Surface Enhanced Raman Scattering (SERS) was investigated using 1,2-bis(4-pyridyl) ethylene (BPE) as the probe molecule. While SERS is widely studied for its applications in sensing and imaging, designing and optimizing effective substrates remains a challenge. To better understand and enhance the SERS process in nanoparticles, gold nanospheres, nanotriangles, and nanostars of similar sizes were synthesized and characterized using High-Resolution Transmission Electron Microscopy (HRTEM). Different concentrations of BPE were dropcast on these gold nanostructures. Among suspensions with equal nanoparticle and dye concentrations, the SERS effect was observed to increase in the order of nanospheres < nanotriangles < nanostars. This trend clearly demonstrates that the number of local field hotspots can be controlled to optimize SERS efficiency. The anisotropic nanostructures are attributed to local surface plasmon "hotspots," establishing a clear relationship between surface roughness and SERS signal intensity

c0092

Yield Efficiency In Green And Chemical Synthesis Of Zinc Oxide Nano Particle: A Comparative Study

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Minimization of potential contamination of the environment caused by unreacted metals in green synthesis through high-yield optimization is a challenging one. The present work focuses on the role of the method of extraction of Plectranthus Amboinicus(PA) Leaves through Boil(B), Crude(C), and Hydrothermal(HT) treatments in the yield of synthesized PA-ZnO Nanoparticles(NPs) and on a comparable study with traditional chemical synthesis method. Minimal research addressed this NP yield in green synthesis. With these three distinct extracts, ZnO NPs synthesis was done using the solution combustion method and was characterized for the study of size, surface morphology, purity, and yield attributes. All the three ZnO NPs have given comparable results of quantum confinement(SPR 264, 264.4, and 266nm for B, C, H respectively) from UV-Vis, crystallite size (34,64 and 47nm for B, C, and H respectively) and phase purity from XRD, nearly spherical morphology from SEM, sample purity and comparable yield (87.2%, 72.8% and 77.8% for B, C, H respectively) with chemical ZnO(83.6%) from EDX. Among the three, the Boil method has given a higher yield and smaller particle size comparable to Crude, HT and Chemical methods.

c0093

Solution-Processed CdTe Nanoparticle Memory Device

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In this study we introduce a memory device utilizing Cadmium Telluride (CdTe) Nanoparticles (NPs) as charge charge-storing unit, the whole device is processed at a temperature below 300 ^{o}C. This low-temperature annealing process not only ensures compatibility with flexible and temperature-sensitive substrate but also reduce production cost and thermal budget. The CdTe NPs are spin coated over the dielectric layer (i.e. ALPO), creating discrete charge trapping sites that enhance charge retention of the memory device. A significant memory window of more than 16 V was observed for a voltage sweep of 25 V. This indicate a substantial difference in both program and erase states, and

this can be utilized for multi-bit storage. This work demonstrates the feasibility of low-temperature processed CdTe NPs-based memory devices. The device offers promising route for development of high performance non-volatile (NV) memory technology with enhanced scalability.

c0094

Zinc Ferrite/Polyaniline Nanocomposites for High-Capacity Energy Storage

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Recently transition metal oxides as capacitive electrodes are finding place in supercapacitor. However, low specific energy and poor electrical conductivity are main drawbacks for energy storage applications. We report, Zinc ferrite nanoparticles (ZnF) and ZnF/polyaniline (ZnF/PANI) in the form of a nanocomposite as a better substitute to be the electrode for supercapacitor. These nanocomposites were prepared by sol gel auto-combustion and in-situ polymerization method and characterized by XRD. The XRD pattern revealed the single phase of highly crystalline ZnF nanoparticles and crystalline-amorphous nature of nanocomposite. The surface morphology is studied by SEM which shows cubic structure of ZnF nanoparticles and formation of core-shell of nanocomposite. Capacitance was measured by electrochemical measurements to examine the impact of introducing PANI in ferrite nanoparticles. The specific capacitance value increased due to high conductivity of PANI.

Key words: ferrite nanoparticles, polyaniline, nanocomposites, electrochemical, specific capacitance.

c0095

Effect of Manganese Doping on Optical Properties of $CsPbCl_3$ Nanocrystals

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Due to the distinct optical and electrical characteristics, inorganic perovskites provide a reliable substitute for hybrid organic-inorganic perovskites in optoelectronic applications [1]. Strong interactions between dopant ions and host NC excitons make doping a useful tool for modifying these features [2-3]. The effective production of blue-emitting $CsPbCl_3$ nanocrystals and the deliberate doping of Pb^{2+} sites with Mn^{2+} ions are reported in this work. The ensuing modifications in the characteristics of photoluminescence (PL) were thoroughly studied both pre- and post-doping. A significant color change from blue to pink, accompanied by a prominent peak in the photoluminescence spectra between 550 and 750 nm, was observed [4]. These findings will greatly enhance our understanding of effective metal ion doping for optoelectronic applications. Additionally, they will be crucial in improving our knowledge of the structural and magnetic properties, thereby advancing their potential applications.

c0097

Green Route Synthesis of CuO Nanoparticles utilizing Trema Micrantha Leaf Extracts

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The green chemistry approach for synthesizing nanoparticles has shown great potential as an alternative to the expensive and environmentally harmful chemical methods. In this study, copper oxide nanoparticles (CuO NPs) were synthesized using a green method that utilized the water extract of Trema Micrantha (*Jamaican Nettletree*) leaf as both reducing and stabilizing agents, with copper (II) nitrate trihydrate salt serving as the precursor. Green CuO NPs were characterized using powder XRD and Scanning electron microscope (SEM) images. CuO NPs with several potential uses, particularly in the biomedical field.

c0098

Variation of Structural, Optical Properties of Different Morphological Zinc Oxide Nanostructured Materials with controlled Synthesis Process

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Different morphologies-based zinc oxide (ZnO) nanostructured materials are synthesized using chemical hydrothermal, and sol-gel auto combustion method. The average particle size and morphologies of the synthesized

ZnO materials are adjusted by concentration of the precursors, calcination temperature and process parameters. The structural, microstructural, and optical properties are studied to verify phase purity and corresponding variations w.r.t different ZnO materials. Different measurements like X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier Transform Infrared spectroscopy (FTIR), room temperature Raman and UV-Vis spectroscopy measurements are performed to study the structural and optical properties. The average crystallite size calculated from XRD are in the range of 30-50 nm. The diameter of particles of ZnO samples are calculated from SEM analysis confirms from 100 nm to 2 μm order. Further room temperature Raman measurements confirm the synthesis of phase pure ZnO nanostructured material with all possible Raman modes of vibrations. The variation of optical band gap w.r.t different particle size is observed. The obtained results will clearly elaborate the different tunable properties of zinc oxide with morphology and synthesis process can be used for various optoelectronic.

c0100

Plasmon mediated dimerization of thiazolidine derivatives on silver nanoparticle film unveiled by surface-enhanced Raman scattering

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In this study, the plasmon mediated chemical transformation of thiazolidine derivatives such as Rhodanine (Rd) and thiazolidine-2, 4-dione (TZD) deposited on AgNP film were investigated using SERS. AgNP films on glass substrate, prepared by the wet-chemical method, provide a clean SERS platform, free from additional chemicals typically found in AgNP colloids which may otherwise influence the plasmon mediated chemical reactions (PMCR). The obtained SERS results infer that Rd and TZD undergo plasmon-induced chemical transformation on the AgNP film surface, forming their dimers. The presence of dimer was evidenced by the characteristic SERS peak at 1566 cm^{-1} attributed to νC=C band of the dimer. These finding also suggests that chemical transformation of Rd and TZD monomer to its dimer on the AgNP surface is triggered by the indirect transfer of energetic hot electrons produced by non-radiative decay of plasmon. The use of AgNP film as a SERS substrate provides alternate platform for studying the PMCR by eliminating the influence of any additional chemicals mostly present in AgNP colloids.

c0101

Study of Optical, Morphological and Compositional Properties of CuS Nanomaterial

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CuS nanomaterial was synthesized using the hydrothermal method with EDTA as a surfactant to control particle formation. The optical, morphological and compositional properties have been studied through SEM, EDX, FTIR, UV-Vis, and PL spectroscopy techniques, revealing that the nanomaterial has an irregular shape, a band gap of 1.48 eV, and distinct emission peaks in both UV and visible regions. The study underscores the potential of CuS nanomaterial for applications in optoelectronics.

c0102

Structural Modification Of Liquid Phase C_{60} Through UV Laser Irradiation

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C_{60} and its derivatives exhibit remarkable properties with high potential for applications in super-capacitors, hydrogen storage, nano-electronics, and memory devices. In this study, we focus on the functionalization of C_{60} using a pulsed Nd:YAG laser of wavelength 266 nm impinged on fullerene dispersions in isopropyl alcohol. Our investigation employs various analytical techniques, including Fourier-Transform Infrared Spectroscopy, Raman Spectroscopy, Absorption Spectroscopy, Field Emission Scanning Electron Microscopy, Energy dispersive X-ray analysis, and Transmission Electron Microscopy. These techniques allow us to thoroughly examine the derivatives of C60 resulting from the attachment of functional groups during the laser irradiation process. We elucidate how laser irradiation affects dispersed fullerene in the liquid phase, leading to significant structural modifications of C_{60}.

c0103

Thorough Structural Analysis Of MACE-grown SiNWs And Its Future Prospective

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This research offers an in-depth structural analysis of Metal-Assisted Chemical Etching (MACE) grown silicon nanowires (SiNWs) and explores it in the terms of their potential future applications. A MACE is a powerful technique that enables the growth of silicon nanowires through a chemical etching process facilitated by metal catalysts. The structural characteristics of SiNWs, including their diameter, length, aspect ratio, morphology, and crystallinity, were thoroughly examined using various analytical techniques such as field emission scanning electron microscopy (FESEM), X-ray diffraction (XRD), and Fourier-transform infrared spectroscopy (FTIR). The study highlights the influence of metal catalysts and etching conditions on the structural properties of the nanowires. Additionally, the potential applications of MACE method SiNWs in fields such as electronics, energy storage, and sensor technology are discussed. The findings underscore the versatility of MACE-grown SiNWs and suggest promising directions for future research and technologies.

d) EXPERIMENTAL TECHNIQUES AND DEVICES

d0001

Mechanical property evaluation of Alloy 690 at different strain rates and temperatures

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Abstract. Mechanical behaviour of Ni-based Alloy 690 is characterized at room as well as elevated temperatures (25^0C – 900^0C) at varying strain rates (0.0033 s^{-1} – 3500 s^{-1}). Quasi-static tensile tests at different temperatures are carried out using universal testing machine (UTM) and split Hopkinson pressure bar (SHPB) test setup is utilized for performing dynamic compression experiments at different temperatures. It is observed that thermally activated deformation mechanisms are prevalent at all the deformation conditions investigated here. However, the flow curve of tensile experiments at 0.0033 s^{-1} strain rate and 800^0C display a rapid increase of stress to a peak value followed by a gradual decrease. Microstructural examination using scanning electron microscope (SEM) of the deformed samples at 0.0033 s^{-1} strain rate and 800^0C reveals dynamic recrystallization in the alloy, which is not present in the samples deformed in compression at high strain rates and high temperatures. This signifies a change in dynamic recrystallization temperature of Alloy 690 with increase in strain rate.

d0002

Study of effect of loading rate on plastic deformation behaviour and fracture toughness of SA516Gr70 steel

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Mechanical properties of material are known to vary with rate of deformation. For stress analysis and structural integrity assessment of structures subjected to high rate of deformation these properties are necessary. Radioactive material shipping cask is such a structure which has to clear the regulatory requirement of 9m drop test. FE analyses of such structures are carried out to determine the worst drop orientation. As such drop tests are an impact event, numerical simulation requires data at deformation rates that are of 2 to 3 order higher compared to that of quasi-static deformation rate. Considering this, deformation and fracture studies of SA516 Gr. 70 steel has been carried out at deformation rate of 500 mm/min in this work. SA516Gr.70 steel is a pressure vessel that is also used for outer shell of lead-shielded cask. The material has ferritic-pearlitic structure and finds a wide application for fabrications of casks for transport of radioactive materials in nuclear industry, pressure vessels and piping etc.

d0005

On The Optical Response of a MgZnO/ZnO HEMT

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Abstract. This article analyzes and reports the optical sensitivity of a MgZnO/ZnO based high electron mobility transistor. An analytical expression of threshold voltage has been developed under the optical illumination considering a new theoretical approach. Further, a new theoretical model of the drain current of a MgZnO/ZnO HEMT has been developed considering the modulation of sheet carrier density. It is observed that the saturated drain current has been shifted by 14.7 % from the dark drain current when no gate bias is applied. In addition, the threshold voltage also shows a significant sensitivity on optical illumination.

d0006

On the Thermal Sensitivity of a GaN MODFET for High Field application

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This paper represents a temperature dependent theoretical model of a GaN Modulation doped field effect Transistor (MODFET) operated at high electric field, under electron velocity saturation. A simple analytical model has been developed to evaluate the DC parameters of the device such as drain current and threshold voltage as a function of mole fraction and ambient temperature. It is observed that the device current is significantly sensitive to the choice of mole fraction of AlGaN, as well as with the thermal variation of the environment. The device performance is also studied with respect to doping concentration and thickness of the N-AlGaN layer. The thermal sensitivities of drain current and threshold voltage are calculated in order to study the thermal effect more precisely.

d0007

A Method of Aligning CNTs in Nanocomposite Polymer Films

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Abstract. A new method of aligning CNTs in polymeric films involves mixing CNTs and magnetic nanoparticles to the polymer solution and casting the polymer film/ membrane in presence of a moderate magnetic fields, has been developed. Polysulfone – MWCNTs nanocomposite membranes were synthesized and the alignment of MWCNTs was examined by carrying out water permeability and dielectric studies. Water permeability was higher for membranes casted in magnetic field and it increased with an increase in magnetic field.

d0009

Fabrication and Application of P(VDF-TrFE) Copolymer Films for X-ray Detection in Synchrotron Radiation Sources

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In this research, we explore the use of polyvinylidene fluoride-trifluoroethylene (P(VDF-TrFE)) thin films to detect X-rays produced by the synchrotron radiation source Indus-2, using their piezoelectric and pyroelectric properties. The films of varying thickness (30-100 microns) were prepared by solution casting and doctor blading techniques. The X-ray Diffraction (XRD) pattern of these synthesized films confirm their semi-crystalline structure and highlighting the presence of β phases essential for piezoelectric performance. Polarization-Electric Field (P-E) loop tracing showed enhanced ferroelectric behavior with increased thickness. The response of these films were observed using X-ray of energy 12keV. The results indicate that the P(VDF-TrFE) films exhibit promising potential for the use in high-energy X-ray detection, with the capability to operate efficiently under the demanding conditions of synchrotron radiation. The uniformity in thickness and enhanced electrical properties contribute to their robustness and reliability as detectors.

d0010

Development of Nanocomposite Films having Low Dielectric Constant for Microelectronics Applications

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High performing polyimide films are finding increased use for packaging in semiconductor industry. Pure polyimide (PI) films, which are otherwise ideally suited for the above purpose, have high dielectric constant of $\kappa = 3.4$. It is of interest to prepare polyimide films having low dielectric constant (say $\kappa \leq 2.5$) and low levels of water absorption. We have synthesized polyimide /silicic acid (SA) and polyimide/ polyethylene glycol (PEG) nanocomposite films and it was seen that dielectric constant of nanocomposites is much lower than that of pure polyimide. Results of FTIR, dielectric and water uptake studies on above nanocomposite films are reported. It was seen that the dielectric constant for PI-PEG films was 1.17 and 1.29 for additive concentrations of 1% and 5% respectively.

d0011

Multi-Channel Count Rate Meter With OLED Display For Neutron Scattering Experimental Facilities

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Since continuous upgradation of the front -end electronics plays a very significant role in the performance of the instruments, we continuously strive to indigenously develop and upgrade the front-end electronics with state-of-the-art technologies that are available. So, keeping in mind the ever-increasing performance demands and ease of maintenance: we have designed, fabricated and assembled a multi-channel module capable of taking the counts of 3 different channels with OLED display on the front panel for displaying the count rate of each channel. This module which is being deployed in Medium resolution Small Angle Neutron Scattering (MSANS) facility at the attached Guide Tube Laboratory in Dhruva Reactor incorporates the functionality of three different Scaler Discriminator Modules in a single module. This paper describes the circuit and the functionality of the module developed.

d0012

First Results of Grating Based Multicontrast X-ray Imaging Technique at Imaging Beamline of Indus-2

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Conventional X-ray imaging techniques which rely on absorption of the beam provides limited contrast for soft materials and offer limited advantage of advance synchrotron sources in study of samples from diverse research domains. We, therefore, report here development of a single grating based multicontrast imaging technique at X-ray imaging beamline of Indus-2 synchrotron source which uses scattering and refraction of the beam as an image signal. It simultaneously generates absorption contrast, dark field/small angle scattering (SAXS) and differential phase contrast image of the sample from single set of acquired data. The multicontrast images of the sample provide complementary structural details which are not possible with conventional absorption based techniques. We illustrate here simultaneously detection of low density and high density features of the sample with enhanced contrast. The qualitative and quantitative structural characterization of different samples has also been discussed to show the potential of the developed setup.

d0013

Vertically Aligned Hexagonal $MoSe_2$ Nanoflakes for Supercapacitor Applications

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Transition metal diselenides (TMDSs) have been discovered to be great for storing capacities and have a distinct place in supercapacitor research due to their extreme hydrophilicity, honeycomb arrangement, and large surface area. This work used DC-magnetron sputtering to deposit molybdenum diselenide nanoflakes on stainless steel (SS) substrate at room temperature in a regulated vacuum level. The structural, morphological and compositional analysis of the thin film were analyzed by XRD, Fe-SEM, and XPS. TMDSs film of MoSe2@SS was evaluated as active electrode material in aqueous solutions of 1M Na2SO4 at varying sweep rates. The MoSe2 nanoflakes showed a good specific capacitance of 182.2 Fg-1 at a sweep rate of 20 mVs-1. The MoSe2 electrode was found to keep about 97 % of its capacitance even after 5000 cycles.

d0014

Effect of Thermal Stress on Bit Error Rate of 2D and 3D NAND Multi Level Cell Flash Memory

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In this work, impact of thermal stress on the bit error rates (BER) of 2D and 3D multi level cell (MLC) NAND flash devices have been evaluated aiming to enhance structural management and reliability. A series of thermal stress experiment has been conducted to measure bit error rate in both type of memory chip at various temperatures starting

from 40°C to 100°C. The 2D NAND demonstrate BER (0.06 %) than 3D NAND (0.02 %) flash memory for the 6 hrs of baking. The BER Pearson's correlation coefficient (r) is better in 3D NAND with r = 0.86 after baking at 100°C for 30 mins. On the other hand, 2D NAND demonstrate very low correlation coefficient (r) of 0.52. Our findings will help in optimizing the data retention capabilities of NAND flash memory.

d0015

Upgradation of a National Facility: High-Q Diffractometer at the Dhruva Research Reactor

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Upgraded High-Q diffractometer is a conventional neutron diffractometer with high Q_{max} = 17.6 $Å^{-1}$ and caters mainly to understand short range order in glasses, liquids and disordered materials. The salient feature of upgraded High Q diffractometer are: (a) Transition from a flat Copper monochromator to a vertically focusing monochromator, resulting in a flux increase at the sample position, along with the option of four wavelengths. (b) Adjustment of beam collimation before the monochromator by using Söller collimators with 5', 10', 20', and 60' divergences, providing multiple resolution options, (c) It can be used in different modes. On Upgraded High-Q different types of experiments like: smaller time frames and smaller samples can be studied (~1g); isotopic substitution experiments can now be done to obtain partial structure factors; ionic hydration studies can be studied for Salt solutions using isotopes; time resolved diffraction and Pair Distribution Function analysis are possible.

d0016

Mathematical Modeling of Vertical Focusing Monochromator

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Vertical neutron Focusing Monochromator (VFM) with focusing range of 1m to ∞ contains 13 No. of single crystal Cu/Ge mirrors, arranged vertically to form a virtually seamless concave reflecting surface to the incoming neutron beam to accurately focus the same to higher intensity on sample to conduct physics experiments. These mirrors independently rotate about backlash free frictionless hinges as modules of different gradients to form concave mirror. These mirrors are actuated by synchronized cams with various gradients mounted on motorized single common shaft. Mathematical model to derive the cam profiles for various gradients, development of relations between common shaft actuation (i/p) and focusing distance (o/p), work space optimization for sensitive working of instrument and augmentation of the range of instrument are presented in this paper.

d0017

Studying the Electrical Properties of Nanostructured TiO_2-Based Diodes And Understanding The Effect of Morphology

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We fabricated Ag/TiO_2-Nanorods (NR)/FTO and Ag/TiO_2/FTO Schottky diode devices in this study. Two devices were prepared, nanostructures (only nanorods) and nanostructures (with nanorods and nanoflowers). These nanostructures were synthesized via hydrothermal synthesis on the FTO substrate at varying temperatures. The electrical properties of the Schottky diode device were measured using the B1500A Semiconductor Parameter Analyzer. The diodes ideality factor (η), Barrier Height (φ_b), and Series Resistance (R_S) were calculated using the Thermionic Emission Model, Norde's function, and Cheung's function. According to our results, both devices showed good rectifying behavior. The device with only nanorods improved the ideality factor and barrier height. Hence, these TiO_2 nanostructures can be used to make diodes.

d0018

Spatial Beam Profile across a Spatial Light Modulator in Holographic Optical Tweezers

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We present a simple technique to determine the laser beam profile across a spatial light modulator (SLM) to generate structured light, in particular holographic optical traps. The optical trap generating algorithms use incident beam profile over the SLM as an input to generate optical traps or any desired pattern of light. In general the incident laser beam is assumed to be centered on the spatial area of SLM. In practice it is difficult to ensure the beam centering on the SLM with a resolution down to 10-15 µm, the pixel pitch of SLM. We present here a method to determine the laser beam profile, the beam center location on the SLM and also demonstrate the effect of different beam center locations on trap uniformity. The method allows generation of optical traps with any arbitrary laser beam profile.

d0019

Temperature Dependent Vibrational Studies on $DyTaO_4$ Synthesized in M′ Fergusonite

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Technologically important rare earth orthotantalate $DyTaO_4$ has been synthesized in M' Fergusonite phase using solid state reaction route. Single phase formation of the compounds is confirmed by analyzing powder x-ray diffraction data and Raman spectroscopic technique. Experimentally observed unit cell parameters and Raman modes have been corroborated with DFT based first principles simulations. High temperature Raman measurements performed on synthesized compound indicates stability of ambient monoclinic phase up to 600 º C.

d0020

Analog Switching and Synaptic Behavior in MoS2/NiMnIn for Bio-Inspired Neuromorphic Computing

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The present study reports a flexible ReRAM device of MoS_2 nano rod reactively sputtered over stainless-steel(S.S.) substrates via D.C. magnetron sputtering. The Cu/MoS_2/NiMnIn/S.S. heterostructure manifests the gradual switching with a high OFF/ON ratio of ~ 100, large endurance (5000 cycles), and retentation(5000 s) characteristics. The resistance versus temperature confirms the metallic filament formation in a low resistance state and semiconductor behavior in a high resistance state. Moreover, the long-term potentiation (LTP) and long-term depression (LTD) characteristics with excellent linearity are obtained using an identical pulse. The phase change characteristics of NiMnIn generate strain in the interface of NiMnIn and MoS_2. It manipulates the conductivity of synaptic functionality. The magnetic enhances the linearity of LTP and LTD.Furthermore, the flexible ReRAM device is tested in no-bending tensile and compressive bending modes. It shows excellent stability of LRS and HRS during bending mode. Artificial devices mimic the biological memory synapse, which is essential for neuromorphic computing.

d0021

Visible-light Effect on CV-Characteristics in Transparent MOS Device

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The core of today's semiconductor technology lies in solution-processed charge trapping Metal-Oxide-Semiconductor (MOS) structures, often hindered by high interface state densities. A spin-coated transparent MOS device has been fabricated on a silicon substrate using ALPO and IGZO. The effect of light illumination on the devices at different frequencies has been measured. A significant shift of CV curve is observed in the inversion region under the illumination of light. The shift of the capacitance due to illumination of light are varied from 32.5 pF to 1.8 pF for the AC signal frequency of 100 kHz to 1MHz. These findings enhance the understanding of light's interaction with MOS structures, crucial for optimizing optoelectronic and memory devices.

d0022

Comparative Study of BF_3 Based Neutron Detectors with Cylindrical and Cuboid Geometry Using COMSOL FLUKA and FLUKA Software

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Abstract. Neutron proportional counters commonly use coaxial cylindrical geometry for advantage of symmetry in electric field distribution and for use in isotropic neutron field. In case of BF_3 filled neutron detectors, electron attachment plays role in high pressure compatibility that determines the sensitivity of a detector. Detectors with complex geometry such as square cross section and array of multitubes is useful to suppress recombination. The square geometry is analyzed for electric field distribution and neutron detection sensitivity. Multiphysics software COMSOL is used for defining detector geometry in 2D mode and simulate electric field distribution in sensitive region of detector. Data obtained from simulations will reflect the shape of pulse height distribution resulting from neutrons. FLUKA software is used to accurately simulate the neutron sensitivity of a detector with coaxial and square cross section geometry of interest. A comparative analysis of multitube-based cylindrical and parallelepiped geometry for BF_3 filled neutron detectors is presented.

d0023

Mn_3O_4 Nanostructures-Based RRAM Devices

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Resistive switching (RS) phenomenon-based memory devices (RRAMs) are considered to be the memory of the future era due to their simple structure, ultrafast switching, low fabrication cost, and less power consumption, etc. Two Mn_3O_4 nanostructure-based Al/Mn_3O_4/FTO RRAM devices were fabricated using Aluminum and FTO as top and bottom electrodes. The first RRAM device was construed by sol-gel synthesized Mn_3O_4 nanoparticles and shows a forming-free feature. The second type of RRAM device was fabricated using spin-coated Mn_3O_4 thin film, which obtains a gradual RESET feature.

d0024

Small-Angle X-Ray Scattering Investigations of Co and Ni substituted Ru-layered double hydroxides

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The catalytic performance and the supercapacitor efficiency of layered double hydroxides are known to depend on their microstructure. In this work, we used non-destructive x-ray scattering technique to get better insight of the structural characteristics of Co and Ni substituted Ru-layered double hydroxides. We found the samples consist large size voids of size ~ 75 nm in the doped samples as compared to ~ 85 nm in the un-doped one. The pores have rough boundaries with subtle differences in the extent of roughness among the samples. They also consist small size particles (4-5 nm) showing compact mass fractal features. The variations in the microstructure are expected to show significant difference in the adsorption performance and hence the energy storage capacity.

d0026

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The rare-earth titanate Gd_2TiO_5 belonging to the Ln_2TiO_5 (Ln= lanthanide element) system has been synthesized via conventional solid-state reaction route. The XRD measurement has confirmed the phase purity of the sample and Rietveld refinement has been performed to extract the crystallographic information about the material. To investigate the optical properties temperature-dependent optical measurements have been performed using UV-VIS spectroscopy. The optical band gap was found to decrease with the temperature indicating electron-phonon interactions could be one of the possibilities. To estimate this, the strength of electron-phonon interactions was measured by fitting the band-gap data with the Bose-Einstein model.

d0027

Fabrication of Simple, Low-Cost and Flexible Graphite-based Thermocouples on Paper

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Temperature is an important parameter in biological bodies and industrial applications. Also, it is important to measure and monitor to check the human body condition and industrial apparatus. In all, the application temperature has been measured by the thermocouple. In this study, first, we synthesize graphene and HB, 6B paint and characterize it with XRD and Raman, which shows the graphitic nature of the samples. We measure its electronics and thermal transport properties. The difference in the Seebeck coefficient motivates to fabrication of thermal sensors. Here, we fabricated three different thermal sensors containing HB, 6B paint, graphene traces and pencil traces. The maximum sensitivity of ~18 μV/K is shown by graphene/pencil traces and graphene trace/HB paint.

d0028

Design of Enclosure Chamber of Large 2D PSD for SANS Diffractometer at Dhruva Reactor

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Small angle neutron scattering experiments require efficient neutron detectors forcovering scattering angle of interest. Isotropic scattering samples are often analyzed using linear 1D position sensitive detector (PSD) intercepting the diameter of the scattered spectrum. Multiple 1D PSDs in fan-like arrangement are must to observe the signature of anisotropic scattering samples, with significant dead regions, however 2D PSD shows the advantage of covering entire area of scattered neutron indicating better statistics as well as access to smaller Q (large length scale). A 2D PSD for neutron scattering is being developed as an import substitute. It has sensitive area of 640 mm × 640 mm and is based on multiwire geometry, ^{3}He gas filled and delay line position encoding. Scaling up of the hardware enclosure considering neutron transmission and permeability of ^{3}He gas are challenges. Design features of gas enclosure chamber, neutron detection efficiency, position encoding and position resolution would determine the success of the 2D PSD development. In this work, the design of enclosure chamber for vacuum and high-pressure tolerance is presented.

d0029

Conceptual design of an innovative shock absorber for possible application in Dhruva reactor

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Abstract. *The innovative concept of extrusion tube as a part of existing shut-off rod (SOR) of Dhruva reactor assembly is developed here. This modification in SOR will absorb drop energy under postulated event of drop of SOR into the guide tube without damaging the tube. Effectiveness of SOR under postulated drop event is evaluated using explicit FE simulations of entire SOR assembly and verified experimentally in Drop Weight Tower machine. It is found that the modified SOR is functioning in intended manner and guide tube remains in elastic condition throughout the postulated event of SOR drop into the guide tube, irrespective of working of existing emergency springs inside the guide tube. New concept of modified SOR can be used as SOR in Dhruva reactor.*

d0030

Indigenous Development of a Closed Cycle Refrigerator for Raman Spectroscopy

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A closed cycle refrigerator has been developed for use in a micro-Raman spectrometer. This work was taken up as indigenous development as import substitution. The set-up has been tested down to 4.2 K. The cool-down time, the temperature stability as well as the mechanical stability have been found to be encouraging. This development of the cryostat will facilitate Raman spectroscopic measurements at temperatures from 4.2 K to 300 K, to probe interesting phonon assisted phenomena condensed matter.

d0031

Sealed D-T Neutron Generator for Borehole Logging and Bulk Material Characterization

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The paper presents design, operational principles, and applications of a compact neutron generator, developed indigenously, which provides a reliable source of fast neutrons for material characterization. The sealed D-T neutron generator offers enhanced safety, portability, and operational efficiency compared to traditional neutron sources. It enables real-time, in-situ measurements of elemental compositions and densities of geological formations and bulk materials. This paper also describes two different applications of this neutron generator. In the first application, we have used Prompt Fission Neutron (PFN) technique for precise identification and quantification of uranium deposits by measuring the prompt fission neutrons. The second application highlights bulk material characterization using neutron-induced gamma-ray spectroscopy, such as in coal to quantify moisture and carbon content, and determine its gross calorific value. Both these experiments were carried using indigenously developed 14.1 MeV D-T neutron source with yield of 5x10^7 n/sec operated in pulsed mode.

d0032

Two-dimensional Halide Perovskite Based Highly Stable Memory Devices

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Organic−inorganic halide perovskites (OIHPs) based resistive random-access memory (ReRAM) devices are emerging as a new class of revolutionary data storage devices. Recently, two-dimensional (2D) OIHPs have stimulated significant interest for ReRAM applications due to their structural diversity and enhanced stability. This study reports on the resistive switching (RS) characteristics of devices constructed with pure 2D Ruddlesden-Popper (RP) perovskite crystals, specifically $(TEA)_2PbBr_4$ and $(TEA)_2PbI_4$. These RS memory devices demonstrate reliable and reproducible bipolar switching behavior with a high ON/OFF ratio of approximately 10^4. Additionally, they exhibit excellent data retention over 10^4 seconds and robust endurance, maintaining performance through 200 cycles. The temperature-dependent RS behavior was analyzed, revealing insights into the formation and dissolution of conductive pathways under an external electric field. Furthermore, the RS properties of the 2D RP perovskite-based memory devices are stable for over 45 days under ambient conditions. These results underscore the potential of 2D perovskite-based ReRAM devices for advanced logic applications, highlighting their stability and performance in environments.

d0033

Comparative Luminescence Study of Scheelite and Wolframite Tungstate Ceramics

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A comparative study of luminescence properties of scheelite (AWO_4, A = Ca, Sr, Ba) and wolframite (AWO_4, A= Mg, Zn, Cu) tungstate ceramics prepared via the conventional solid-state reaction technique was conducted. The crystal structure confirmation and phase identification were done by X-ray diffraction (XRD) pattern followed by Rietveld refinement analysis. Thermoluminescence (TL) response from room temperature to 350 °C of all the prepared samples was investigated after β-irradiation at heating rate of 5 °/s. A distinct glow peak of second order was evident in case of scheelite tungstates, but not for wolframite tungstate. The radioluminescence (RL) response recorded upon X-ray excitation exhibited a broad spectrum for $CaWO_4$, $SrWO_4$, $MgWO_4$, and $ZnWO_4$ ceramics in the range 400 to 700 nm. $BaWO_4$ and $CuWO_4$ showed no significant RL intensity at room temperature. The insights gained from these results highlight the use of these materials in radiation dosimetry and detection applications.

d0034

Error identification and mitigation in fast voltage-sweeping emissive Langmuir probe measurements

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We report the error encountered and its mitigation in the emissive Langmuir probe measurements due to the application of fast voltage sweep of ~ 1 kHz. In these measurements, an electronic circuit's sensitivity is crucial because, when the plasma potential, ϕ_{pl} is directly determined using the emissive Langmuir probe, even a minute error will have significant impact on estimation of the electric fields. When it comes to error-free measurement in EP experiments, the key error in the measurements arises mainly due to the cable capacitance of widely popular RG58 coaxial cable used for data collection. The error has been mitigated using a suitable dummy cable. Efficacy of capacitance compensation using dummy cable configuration is tested and the error is significantly reduced as compared to the single cable configuration. The results highlight the limitation of circuitry composed of semiconductor and electrical components in practical application.

d0035

Temperature dependent electrical transport properties of W/WS_2 junction

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In the past decade, transition metal dichalcogenides (TMDs) have become a major focus of research due to their layered structures and tunable band gaps. Tungsten disulfide (WS_2), in particular, is an intriguing material for optoelectronic and electronic device applications. We have synthesized a WS_2 thin film on n-type silicon (100) employing the DC sputtering technique, which ensures uniform and homogeneous growth. Subsequently, we fabricated a 1mm diameter tungsten (W) contact onto the WS_2 thin film utilizing a shadow mask and DC sputtering. We measured the current-voltage characteristics of W/WS_2 junction over a temperature range of 270-350K to investigate the current transport mechanism. The results indicate that the current transport is not solely governed by thermionic emission. The I-V-T measurements are utilized to extract Schottky parameters, revealing that the ideality factor decreases while the barrier height increases with temperature. Also, the deviations from thermionic emission can be assessed by measuring the standard deviation from homogeneity.

d0037

Efficient Transmission Gate with Charge Plasma Doping: A Simulation Study

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In this article, we present design and simulation study of a novel transmission gate that utilizes charge plasma doping to eliminate the requirement for physical doping. In contrast to conventional CMOS transmission gates, which normally require two transistors for the NOT gate and another two for signal transmission, our proposed design functions with just two silicon blocks. This design significantly streamlines the structure while still retaining its functionality. We employed Silvaco ATLAS to run detailed device-level and mixed-mode simulations to assess the performance and features of the proposed doping-less transmission gate. The voltage transfer characteristics (VTC) curve, transient analyses of the NOT gate, and transient and mixed-mode analyses of the final transmission gate are all important studies. Additionally, we present the carrier concentration profiles induced by charge plasma doping. The results demonstrate that our doping-less design not only reduces the complexity and transistor count but also achieves robust performance, making it a promising candidate for future integrated circuit applications.

d0040

Micro-Kelvin Laboratory at BARC for Physics Research at Ultra Low Temperature

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We report the measurement of an ultra-low temperature of 480 microkelvin (μK) in our laboratory after using the technique of adiabatic nuclear demagnetization on a 5 kg Copper block, which was attached to a dilution refrigerator through a superconducting switch made from aluminium. This experiment represents a significant advancement in low-temperature physics, demonstrating the efficacy of nuclear demagnetization techniques and the stability of superconducting switches in maintaining ultra-low temperatures. Accomplishment of such a stable environment of ultra-low temperature has the potential of implementation and utilization in future low-temperature experiments and applications relevant in the field of quantum computing.

d0041

First Polycrystalline Diamond-based XAFS Experiments At Indus-2

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The scope of Polycrystalline Diamond-based High Pressure XAFS experiments at Indus-2 has been explored. Glitch-free high-quality spectra were generated for Zr foil, which inspires us to undertake challenging XAFS problems under high pressure.

e) SINGLE CRYSTALS, GLASSES AND AMORPHOUS SYSTEMS

e0001

Analysing the changes observed in Neutron diffraction peaks of $Cs_6H(HSO_4)_3(H_2PO_4)_4$ crystal as it undergoes Deterioration

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Single crystal neutron diffraction investigation on superprotonic crystal $Cs_6H(HSO_4)_3(H_2PO_4)_4$ belonging to $CsHSO_4$–CsH_2PO_4–H_2O solid solution system was undertaken by us earlier, it was found that the crystal underwent a spontaneous deterioration after a few days of data collection most likely due to change in ambient condition. Structure for the crystal was obtained before as well as after deterioration and it was found that the unit cell of the crystal had contracted due to strengthening of the O-H---O hydrogen bonds of the crystals. We report here how the above mention change in the hydrogen bonding affected the diffraction intensities as well as peak shapes for the crystal, Williamson-Hall analysis is performed to estimate the lattice strains introduced due to this change in hydrogen bonding network. Finally the changes in the potential energy contour of the O-H---O hydrogen bonds have been modeled and expected consequences of these changes on proton conduction discussed.

e0002

Structural and Magnetic Properties of Nd_2TiO_5 Single Crystal

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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.

e0003

Investigating the Role of Strontium on the Bioactivity of Silicate Glass and the Effect of Doping Fe

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Bioactive glasses are playing crucial role in bone tissue engineering applications as they are used as temporary template for tissue regeneration. With regards to their design some issue still remains unfolded. Strontium is one of the trace elements that plays role to slow the breakdown of old bone. In the present study strontium silicate glass doped with Fe was synthesized by conventional melt quenching technique. From Raman spectra, it is identified that the glass doped with Fe exhibited higher relative percentage of Q^2 silica species indicating enhanced bioactivity as well as the formation of silanol (Si-OH) groups. In vitro study soaking pellets of glass powder in simulated body fluid for 3 ,7 and 21 days showed the formation of Hydroxyapatite (HAp) crystals. In the case of pellets immersed for 21 days, crystalline phases of HAp became more prominent enhancing their bioactivity. Enhancement of bioactivity can be achieved by tailoring the composition of Fe and Sr to meet specific performance in biomedical applications.

e0004

Growth of Single Crystal Diamond Substrates Via Welding- Assisted Microwave Plasma Enhanced Chemical Vapor Deposition

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Lab grown single crystal diamonds (SCDs) offer unrivalled hardness, a wide range of optical transparency, and supremely high thermal conductivity reliable materials to be a part of devices run at high frequency, temperature, and power. Effective synthesis techniques are essential in enhancing the potential applications of high-quality SCDs. This study aims to decrease the thermal contact resistance between diamond seeds and the molybdenum holder by utilizing welding material. Quality of grown diamond substrates (plates) were assessed by Raman spectroscopy. In the Raman spectra, a peak near 1332 cm-1 called the first-order Raman peak confirms the diamond phase of grown crystals.

e0005

Synthesis and Characterization of Bismuth Doped Borate Glass for nuclear radiation shielding application

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Here we report the synthesis of $(100 - x - 2y)B_2O_3 - xBi_2O_3 - yCdO - yAgNO_3$ glass system for possible nuclear radiation shielding application. The concentration of Bi_2O_3 was varied from 5 to 45 mol% and corresponding γ-ray shielding property is studied. CdO was used for enhancing neutron shielding properties of the glass and in some cases $AgNO_3$ was replaced by LiOH to improve its neutron attenuation property keeping the concentration between 6 mol% to 10 mol%. The X-ray diffraction analysis was done to confirm the amorphous nature of the glass samples prepared. The densities of glass with 10 and 45 mol% of Bi_2O_3 have been found to be 6.0 and 6.49 g/cc, respectively. The optical transparency measurement of the sample shows that it is more than 50% transparent above 441nm wavelength. The initial study demonstrates that at 25 mol% of Bi_2O_3 the attenuation coefficient (μ) of the glass is $0.24\ cm^{-1}$ at 1.275 MeV of γ-photon energy, much more than aluminum (0.136 cm^{-1}) and also agrees with corresponding WINXCOM and Geant4 simulation results. The half and tenth value layer thicknesses were measured as 2.89 cm and 9.59 cm for Bi_2O_3~25% and 4.72 and 15.66 cm for Bi_2O_3~5%, respectively. Further work on neutron shielding properties is in progress

e0006

Single Crystal Growth of Sn doped Ca_2RuO_4 using Optical Floating Zone Technique

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We present the single crystal growth of Sn doped 4*d* transition metal oxide Ca_2RuO_4, a single layer compound of Ruddelsden-Popper (RP) series. In the literature, this series of single crystals have been synthesized using techniques such as flux method and optical floating zone technique. Here, we employ the optical floating zone technique by utilizing RuO_2 as a self-flux to grow single crystal, while analyzing the challenges encountered in the midst of the growth process such as molten zone formation & stabilization, and gas mixing ratio. Further after the growth, evolution of those grown crystals with time were tracked for 6-7 days. The grown crystals were characterized by powder x-ray diffraction, back-reflection x-ray LAUE, energy dispersive x-ray analysis (EDX), and x-ray rocking curve analysis. The crystals cleaved surface are examined by optical light microscope. The grown crystals crystalize in orthorhombic structure (*Pbca*) with distorted RuO_6 octahedra, where Ru atoms are placed at *4a* special Wyckoff-position site.

e0007

Growth and Characterization of Semi Organic Amino Nitrate Crystal (GPC) For SHG Application

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The mixed amino-nitrate (GPC) crystals were grown from saturated solutions using the slow evaporation technique with a molar ratio of 3:0.5:0.5. Transparent, elongated crystals of significant size (17 x 9 x 6 mm^3) were obtained in about 3-4 weeks. The solubility of GPC crystal in water was determined. The grown crystal belongs to the orthorhombic system with cell dimensions a= 21.2907 a.u, b= 7.7940 a.u, and c= 6.5552 a.u. Intense peaks were

recorded at 2θ = 20° to 40° with a maximum intensity of around 2292 on plane (6 0 0), and the unit cell volume is 1082.77 a.u³. FTIR studies verified the presence of fundamental groups. UV studies indicated a wide transparency window useful for optoelectronic applications. The optical second harmonic generation (SHG) conversion efficiency of GPC crystal was evaluated using an Nd-YAG laser (1064 nm). Additionally, photoconductivity and I-V characteristics were examined.

e0008

Hardness, Thermal and Structural Properties of Sodium Barium Alumino-borosilicate Glasses

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Sodium barium alumino-borosilicate glasses of composition: $5Na_2O$-xAl_2O_3-$7.5B_2O_3$-$(47.5-x)BaO$-$40SiO_2$ (x = 7.5 and 10 mol%) were prepared by melt quenching in a temperature range of 1400-1500°C. Glass samples were characterized by differential scanning calorimetry. The Al-O and B-O coordination environments were determined by ^{27}Al and ^{11}B Magic angle spinning nuclear magnetic resonance (MAS-NMR) spectroscopy. The short-range structure of glasses consists of AlO_4, AlO_5, BO_3 and BO_4 units. Glass density was measured by Archimedes' method and the hardness of samples was measured by Vickers indentation technique. It is found that on increasing Al_2O_3 content, glass transition temperature (midpoint value) decreases from 758 to 755°C. Hardness decreases from 4.67 to 4.57 GPa and density decreases from 4.02 to 3.87 ± 0.01 $g \cdot cm^{-3}$. The fraction of tetrahedrally coordinated Al species decreases slightly and five coordinated Al increases on increasing alumina concentration and there are no hexa coordinated Al (AlO_6) units in these glasses.

e0011

Understanding the Local Structure of Rare-Earth Tellurite Glasses through Neutron Diffraction

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Total neutron diffraction was used to measure the structure factors of Rare-earth (R = Ce, Pr, and Nd) Telluride glasses. Analysis was carried out using isomorphic substitution method and difference functions were sine-Fourier transformed to determine the separate correlations involving R3+ cations from the matrix. The average R-O bond length is 2.43(2) Å and the average coordination number varied from 5.6(1) to 5.7(4) for different rare-earth ions. The similarity in the spread of Te–O bond distribution for rare-earth tellurite glasses of identical composition, combined with the determination of rare-earth coordination numbers using isomorphic difference functions of measured S(Q) data, strongly suggests that the tellurium environment in rare-earth tellurites is not influenced by the modifier cation.

e0012

Soft X-ray Energy Calibration in BL-03 Indus-2 with an In-house Grown Potassium Acid Phthalate Crystal

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Photon energy calibration of soft x-ray monochromator is of the utmost importance for precise measurements at a synchrotron beamline. Conventional methods based on absorption edge measurements using gas cells or metal foils, face limitations such as limited energy points, contamination issues and associated experimental difficulties. Potassium acid phthalate (KAP) crystal has sufficiently large d-spacing (1.3315 nm) and therefore can be used for photon energy calibration in the soft x-ray region. In the present study we have calibrated the soft x-ray reflectivity beamline, BL-03 at Indus-2, having photon energy range of 100 eV to 1500 eV, using an in-house grown KAP crystal. We have measured the angular positions of Bragg peaks corresponding to unknown incident photon energies and then applied the Bragg law to determine the actual values of incident photon energy. Below 800 eV energy region, higher order Bragg peaks are used to overcome the limitations caused by lattice spacing of the KAP crystal.

e0014

Evaluating the role of CuO on structural and optical properties of Na_2O-P_2O_5 glasses

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The melt-quench method was used to synthesized the composition of $50P_2O_5$-(50-x)Na_2O-xCuO, where x = 0, 1, 3, and 5 mol%. When CuO is added in place of Na_2O the density of the as-prepared samples is increasing from 2.36 to 2.43 g/cm^3. The amorphous nature of the developed glasses is confirmed by X-ray diffraction. The influence of adding copper on optical properties and the structural changes in the phosphate network were examined by a various of characterization techniques. It is observed that upto 3 mol% copper was act as a former which leads to polymerized the polyphosphate glass network. However, at higher concentration i.e., above 3 mol%, CuO act as a modifier and induces a subsequent depolymerization of the phosphate chain.

e0015

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. Here we report a systematic study on Fe doped Bi_2Se_3 single crystals grown by vertical Bridgman technique using X-ray diffraction, angle resolved photo electron spectroscopy, X-ray near edge structure and extended X-ray absorption fine structure measurements. The experimental observations have also been corroborated with the results of theoretical simulations carried out on Fe doped Bi_2Se_3 system by density functional theory based formalism.

e0016

Tellurium Inclusions Characterization and Optimization of Surface Processing Steps for Detector-Grade CdZnTe

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Single crystals of the II-VI group semiconductor material CdZnTe (CZT) were grown using the travelling heater method in an indigenously developed setup. Tellurium was used as a solvent. The growth process was conducted with varied temperature gradients, growth rates, and rotation rates. Wafers were cut, lapped, and polished from the grown ingot using progressively finer Al_2O_3 particles, ranging from 15 µm down to 50 nm. Infrared transmission microscopy was employed to map tellurium inclusions across the CZT wafer, and the correlation between the size and number density of Te inclusions and growth parameters was studied. The wafer was then chemically etched to remove the damaged layer caused by cutting and mechanical polishing. Various alternative chemical etching solutions were studied to determine which were best suited for CZT, offering better etching potential and controllable etching rates. The solution comprising 5% potassium dichromate, 10% nitric acid, and 85% ethylene glycol is a promising alternative to the 2% Br-methanol solution, which has high toxicity and volatility.

e0017

Effect of induction power supply frequency on the growth of Germanium single crystal

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Initial crystal growth simulation to simulate temperature profile during growth of germanium single crystal by Czochralski crystal growth technique is performed using COMSOL multiphysics software based on finite element analysis technique. The effect of susceptor thickness and frequency of induction power supply (~10 kHz and ~50 kHz) on the melt temperature profile is studied. It was found that for a susceptor thickness of 5 mm, direct coupling of induction power with melt is 5 times more in case of 10 kHz causing higher melt temperature than the graphite susceptor. This may result in melt temperature fluctuation causing growth instability as observed in few growth runs carried out with new 10 kHz induction power supply.

e0018

Evaluation of Light Induced Metastable Defects in $Se_{90}Ag_6Sb_4$ Amorphous Chalcogenide Thin Films by Space Charge Examination

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A well-known Space charge analysis (SCA) is employed for the analysis of defect density for different illumination time, and quantitatively found Light induced metastable defects (LIMD) on the Se90Ag6Sb4 thin films of Amorphous Chalcogenide Materials (ACMs). The outcomes show that density of defect states (DOS) raises with illumination time i.e. generation of LIMD took place. On the basis of LIMD suitability of optoelectronic applications can be explored further.

e0019

Judd Ofelt Intensity Parameters of Europium Ion Doped Borate Glasses for W-LED Applications

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Boro Lithium Europium glasses are prepared by the melt quench method. According to Hruby's Criteria value, the prepared sample possesses high thermal stability. X-ray diffraction spectra and the physical property metallization reveal the amorphous and metallic nature of the glass samples. The high density and refractive indices of these glasses substantiate their suitability for use in optical systems. The absorption spectra of this optical material reveal that the maximum absorption lies in the range of 393nm. Judd-Ofelt results obtained from UV-VIS absorption measurements have been applied to photoluminescence spectra to evaluate radiative properties like Ω_2, Ω_4, Ω_6 values are compared. The obtained results show that the optical properties of the glass sample EuB1 to EuB5 are found interesting for applications in optical systems. The CIE plot shows that the produced glass sample EuB1 to EuB5 emits white light. So, these glasses are utilized for white LEDs.

e0021

Effect of Gamma Irradiation on Shielding, Optical and Structural Properties of Barium Zinc Borosilicate Glasses

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We report studies on preparation and characterization of lead-free CeO_2-BaO-ZnO-B_2O_3-SiO_2 glasses for possible use as radiation shielding windows (RSW). Glass disks were irradiated with ^{60}Co source and evaluated for their shielding, optical, structural and mechanical properties. Glasses showed transparency higher that 80% in visible range. Radiation induced absorption was found to be lower for cerium doped glass. Effect of different dose rates showed no significant changes in absorbance value. Hardness value reduced with the addition of ceria and also after irradiation due to the

formation of defects. Increase in voids/free volume was revealed form Positron Annihilation Lifetime Spectroscopy after irradiation.

e0023

Effect of grain selector on scintillation properties of CsI:Tl single crystal (Size: Ø75 mm x Length:100 mm) grown by Bridgman Technique

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CsI is a well-known scintillator, used for decades in various applications in fields such as medical imaging, nuclear physics research, and homeland security. For high-energy gamma radiation or low-count events, the use of large-sized scintillators is imperative. Growing large crystals poses challenges, such as restricting polycrystalline growth, controlling of uniform temperature profile and achieving uniform dopant distribution throughout the crystal. In this study, CsI:Tl crystals were grown using the Bridgman technique with carbon-coated quartz crucibles, both with and without a grain selector. The application of the grain selector was found to improve single crystal qualities and uniformity in dopant concentration, resulting in enhanced scintillation characteristics, particularly in terms of the detector's energy resolution.

e0025

Growth and characterization of Bismuth Germanate (BGO) single crystals in indigenously developed Czochralski puller

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The Czochralski technique is widely used to grow single crystals of semiconductors like Si and Ge, as well as oxides such as YAG, YAP, LSO, BGO, GGAG, and many more. The Czochralski puller is a highly specialized system, and until now, all such equipment had to be imported into India at a high cost. Additionally, the limited availability of maintenance services for these imported pullers has hindered the advancement of crystal growth development in India. Therefore, the indigenously developed Czochralski puller is necessary to enable self-sufficiency. By reducing dependency on imported equipment, it supports technological self-reliance and cost-effectiveness in the industry. The indigenous development of the Czochralski puller has been initiated at BARC. In this work, we report that the Czochralski puller has been fabricated in association with a local manufacturer, tested, and commissioned. Furthermore, a BGO single crystal has been successfully grown using this system.

f) SURFACES, INTERFACES, AND THIN FILMS

f0001

Structural and Morphological Evaluation of Reactive RF Sputtered ZrO_xN_y Thin Films as a function of Oxygen Gas Flow Rate

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The main motivation of this work is to develop low-cost, cryogenic sensors which are extensively used for measuring low temperatures (1.5K to 300K) in presence of high magnetic field. It is challenging to record drift free measurement of cryogenic temperature under the presence of magnetic field. At present, commercially available, CERNOX sensors are being used for such applications. In this regard we have initiated our research to develop ZrO_xN_y thin films which is expected to have similar temperature dependent electrical properties as the patented commercial sensors. This work aims to study and analyze deposition temperature in order to tune the electrical properties of ZrO_xN_y thin films. Thin films of ZrO_xN_y with uniform thickness (~ 300nm) were deposited on Al_2O_3 single crystal substrate 300°C using reactive RF sputtering of Zirconium metal target with a combination of Argon, Oxygen and Nitrogen gas atmosphere. The O_2 flow rate was varied from 0 sccm to 0.5 sccm while keeping the N_2 flow rate fixed at 2.5sccm and the Ar flow rate was fixed at 25 sccm. The structural characterization of these films was carried out with the help of x-ray diffraction (XRD), the XRD patterns could be indexed with respect to the reference data of JCPDF # 31-1493 (Fig. 1(a)) for flow rates 0 and 0.2 sccm, confirming them to be single phase. For 0.3 sccm the XRD data shows two phases one conforming to JCPDF # 31-1493 and the other conforming to JCPDF #48-1637. The morphological characterization of these films using Scanning Electron Microscope (SEM) (Fig 1(b, c)) suggest that the films deposited at 0.5 sccm have compact and smooth morphology with smaller grains as compared to the film deposited at 0.2 sccm. It is observed that by increasing the oxygen flow rate from 0.2 to 0.4 sccm, the sheet resistance of ZrO_xN_y films increases (Fig. 1(d)), which can be attributed to the growth of $Zr_7O_{11}N_2$ phase. This is also confirmed from the UV-Vis data which shows that with the increase in oxygen flow rate the optical bandgap increases resulting in increased electrical resistance. Thus, from the experimental results the O_2 flow rate of 0.2sccm showed optimum results. All the results obtained are discussed in details in the manuscript.

f0002

Silicon Surface Energy Modification Using UV, IR Laser and RF Plasma Exposure

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Abstract: To enhance adhesion of gold (Au) on silicon (Si) substrate, systematic surface energy modification techniques such as IR laser, ultraviolet (UV-172 nm) irradiation, and radio frequency (RF) oxygen plasma exposure were employed. The effects of these treatments are analyzed by measurement of water drop contact angle using goniometer and x-ray reflectivity. The water drop contact angle variation and measured surface energy show UV and oxygen plasma treated increases surface energy while IR laser treated decreases surface energy. Hard x-ray reflectivity measurements provided structural (surface roughness, thickness, density) and optical parameters (optical constants: δ and β) of pristine and surface treated substrates.

f0003

Selective Determination of Nickel Ions - Utilisation of Poly-o-toluidine/ Single Walled Carbon Nanotubes Nanocomposite

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Abstract. In this investigation, poly-o-toluidine (PoT) / single walled carbon nanotube (SWNTs) nanocomposite was used for the electrochemical modification of stainless steel (S.S.) electrodes. As the nanocomposite was aimed to

investigate as a sensing element for detection of heavy metal ions (viz. nickel), therefore in terms of selectivity inculcation, it was modified with chelating ligand – Dimethylglyoxime (DMG). The chemical composition of the PoT/SWNTs nanocomposite was studied using Fourier Transformed Infrared spectroscopy (FT-IR) before and after modification with DMG. The electrochemical characteristics of the PoT/SWNTs nanocomposite were studied before and after modification using cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS) to study the electroactive nature of the nanocomposite. The electroanalytical studies were performed by differential pulse voltammetry (DPV) after chemical accumulation of metal ions on the modified nanocomposite to study the influence of pH on detection of metal ions and cross analyte study in terms of the identification of selectivity. A calibration graph was obtained for the concentration ranges, which took place in order to check the sensitivity up to the lower detection limit of the modified nanocomposite electrode.

f0004

Effect of deposition time on chemically synthesized CuS thin film for photodetectors

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In this work, covellite copper sulfide (CuS) thin film has been deposited on the glass substrates by the low-cost chemical bath deposition (CBD) method with 1:4 molar ratio of copper and sulfur at 60 °C with a variation of deposition time 1 hr, 2 hr, and 3 hr. The structural, electrical, and optical properties of CuS thin film deposited at different deposition times have been investigated. XRD confirms the presence of the covellite phase of copper sulfide thin film. Raman spectroscopy reveals a prominent peak at 475 cm^{-1}, corresponding to the vibration of the stretching mode of the S-S bond, which depicts the formation of the covellite phase of copper sulfide thin film. The crystallinity of CuS thin film is found to be increased with an increase in the deposition time. The Hall effect measurement system has revealed the p-type nature of CuS thin film. The current-voltage plot shows the ohmic nature of CuS thin film, indicating a good metal-semiconductor contact. The CuS thin film, deposited for 3 hr, possesses a carrier concentration of 7.4×10^{18} cm^{-3}, and mobility of 29.49 $cm^2/V.s$, which can be a suitable candidate for fabrication of photodetector.

Keywords: Chemical bath deposition (CBD); XRD; Raman; Hall.

f0005

Modifications Of The Structural, Electronic Structure and Magnetic Properties of $PrVO_3$ Thin Films By 100 MeV Au Ion Irradiation

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This study explores the impact of ion irradiation on $PrVO_3$ thin films, examining structural, electronic, and magnetic properties. X-ray diffraction (XRD) reveals stress induction and lattice distortion due to ion track formation. X-ray absorption near edge structure (XANES) confirms the stability of the V^{3+} oxidation state, and extended X-ray absorption fine structure (EXAFS) analysis indicates changes in bond distances affecting the VO_6 octahedra. Magnetization measurements demonstrate reduced saturation magnetization and increased coercivity due to defect formation and partial amorphization.

f0006

The effect of Ar flow rate in annealing on the structural, morphological and mechanical properties of NiTi films

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NiTi films were deposited on Si substrates by RF and DC magnetron sputtering using elemental Ni and Ti as sputter targets. After that the films were annealed at 600 °C with different Ar flow rates to examine the impact of annealing

with different Ar flow rates on NiTi films. It was found that annealing NiTi films at 600 °C with different Ar flow rates can modify their structural, morphological, and mechanical properties. The results suggest that films deposited at room temperature were amorphous and of lower roughness. After annealing with higher Ar flow rates, films become more crystalline and have a higher roughness. The results obtained from XPS also suggest that Ni-rich precipitates such as NiTi, $Ni_{14}Ti_{11}$, Ni, and TiO_2 (metal oxide) layer was formed on the surface of the films. The maximum hardness, elastic strain to failure (H/E) ratio and resistance to plastic deformation (H^3/E^2) achieved in the film were annealed at a lower Ar flow rate.

f0007

Fabrication of Al_2O_3 Nanopore By Anodization Technique for SERS Application

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The synthesis of anodic aluminum oxide (AAO) nanostructures and their morphology has generated significant attention in the field of nanotechnology. The fabrication procedure of anodic aluminum oxide involves a controlled electrochemical process known as anodization. This process transforms aluminum into a highly ordered nanostructured oxide material which is suitable for Surface Enhanced Raman Scattering (SERS). In this work a pure Aluminum foil was two step anodized with voltage variation of 40 V to 60 V for six hours at 1-step and one minute for 2nd step. Samples were then coated with plasmonic gold nanoparticles with spin coating technique. Scanning Electron microscopy and Raman spectroscopy characterization was performed on samples to study their morphology and SERS properties of samples. R6G of different concentration is drop casted on SERS substrate to study the SERS signal enhancement.

f0008

Towards Sustainable Construction Materials: CO_2 Sequestered M-Sand-Cement Blocks

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Abstract. This study delves into the impact of carbon dioxide curing on cement blocks, specifically looking at their microstructure, mechanical strength, and CO_2 uptake. The cube and cylindrical shaped cement blocks were made to test the CO_2 uptake capacity at 0.25 bar and consequent effect on its compression strength. CO_2 curing of cement-M sand blocks were carried at two different water to cement ratios, namely 0.48 and 0.35 at 0.25 bar pressure. Analysis of CO_2 uptake by mass gain method on an ASTM standard block reveal about 12.5 wt.% uptake while retaining a compression strength of 22.1 MPa. We gather evidence from thermal analysis and XRD data that enhanced formation of calcium carbonate takes place when subjected to CO_2 curing. Furthermore, a significant amount of microstructure densifications was observed from SEM analysis. The results indicate that CO_2 curing in M-sand-cement block sequester significant amount of carbon without compromising on the structural strength of the material block. Therefore, CO_2 curing of M-sand - cement blocks offer a sustainable way of utilizing construction materials by mitigating over-all carbon footprint of its production process.

f0010

Panoptic Exploration of Morphotropic Phase Boundary in Gd doped Bismuth Ferrite Thin-Films for Ferroelectric Applications

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Bismuth ferrite (BFO) is a typical example of a multiferroic material. Apart from multiferroic materials, they have the potential to be used in other major applications such as photovoltaics, memory devices, gas sensors, and photocatalysis. A prominent source of these applications is the distorted rhombohedral phase and the relative ease with which the phase can be changed to suit the application. However, it has always had a propensity to leak current and cause unintended phase change. In our work, we employed Gd doping into BFO to enhance its ferroelectric properties. The reason lies in the fact that doping into Bi can reduce the oxygen vacancies created by Bi volatisation and the creation of a morphotropic phase boundary. As Gd is magnetic, this work provides additional dimensions to Gd doping which can potentially be employed in magnetoelectric coupling applications. We observed that 8% Gd

doping provides the best ferroelectric properties which show saturated ferroelectric loops and a maximum polarisation of 19 µC/cm2

f0011

Trap Dynamics in ALPO Capacitive Devices

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Charge-trapping oxides are essential for non-volatile memory storage in electronic devices such as smartphones, laptops, industrial robots, and self-driving cars. However, the performance of memory technology often degrades due to the interface state density between the oxide and the semiconductor. In this work, we demonstrate fully solution-processed Aluminum Oxide Phosphate (ALPO) devices, which exhibit unique memory-like behavior due to intrinsic trap levels. These intrinsic traps cause a distinct hysteresis in the capacitance-voltage (CV) traces, highlighting the devices memory-like characteristics. Our ALPO devices show a charge storage capacity of 1.75×10^{13} cm^{-2}, a low leakage current density of 7.8×10^{-9} A/cm^2, and a low interface trap density (Dit) of 9×10^{10} $cm^{-2}eV^{-1}$, which are critical for high performance. Thermal treatment alters trap density and influences electrical performance, affecting voltage and leakage current. The interplay between carrier transport and electric field effects, driven by interface trap density and gate voltage, offers valuable insights into MOS capacitor behavior. This research underscores the potential of ALPO in enhancing electronic device efficiency and scalability.

f0012

Effect of Stacking of Layers and Variation of Ag Layer Thickness in (Cu, Al)-SnO_2/Ag Layer on Optical and Electrical Properties

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Abstract. The CuAl co-doped SnO_2 single layer, (CuAl)-SnO_2/Ag bilayer of different thicknesses, and (CuAl)-SnO_2/Ag/(CuAl)-SnO_2 multilayer thin films were successfully deposited by the e-beam evaporation method on a glass substrate. The current study examines how varying the thickness of Ag affects the structural, optical, and electrical properties of CAT/Ag thin films. Layer stacking significantly impacts both the electrical and optical characteristics of materials. With layer stacking, both optical transmittance and electrical conductivity increase, reaching maximum values of 67.34% and 3.09×10^4 $\Omega^{-1}cm^{-1}$, respectively. Additionally, increasing the thickness of the silver (Ag) layer further enhances these properties, resulting in an optical transmittance of 57.02% and an electrical conductivity of 1.16×10^4 $\Omega^{-1}cm^{-1}$.

f0014

Improved Decomposition of Carbonized Sucrose Catalyzed by Ceria Nanocuboids

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Ceria nanocuboids have been used to accelerate the decomposition of carbonized sucrose. Carbonization of sucrose was done by annealing at 500 °C under N_2 atmosphere. Structural purity of the ceria was ascertained using X-ray diffractometry, Transmission Electron Microscopy and Selected Area Electron Diffraction. The catalytic influence of the ceria nanocuboids was established by comparing the Thermo gravimetric results of pure carbonized sucrose and that mixed with 9% ceria.

f0015

Investigating Temperature-dependent Raman Spectroscopy and Photoresponse Study of Bi_2Te_3 Thin Film for Optoelectronics Application

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Nanocrystalline Bi_2Te_3 thin films of 800 nm thickness synthesized via the thermal evaporation method were annealed at various temperatures that induced notable changes in both structural and optical characteristics. Structural analysis confirmed the presence of the rhombohedral Bi_2Te_3 phase in the material. The crystallinity was enhanced at increased annealing temperature. Temperature-dependent Raman studies revealed a red shift in the vibrational modes. Morphological analysis insights into the slight agglomeration in the films at a higher annealed state. Photo-response studies indicated an increment in the photo-current with higher annealed films. The observed optimized properties of the films are suitable for various optoelectronic applications, such as absorber layers for solar cells, Infrared devices, and other photo-response applications.

f0016

Structural and Optical Properties of Reactively Sputtered Nanostructured NiO Thin Films for NO_2 Gas Detection

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NiO thin films were fabricated by reactive magnetron sputtering using different O_2/Ar gas flow ratios, for toxic gas detection. The films deposited at room temperature without further annealing were analyzed to be crystalline. The influence of various gas flow ratios on the structural, optical and morphological properties of the films was examined through measurements made with several sensitive techniques namely XRR, GIXRD, FESEM, SIMS and UV-visible spectroscopy. It was found that these nanostructured films were sensitive to NO_2 gas detection at room temperature. Apart from exhibiting a fairly good sensor response, the fabricated NiO films were observed to undergo complete recovery between sequential gas doses of increasing concentration.

f0018

Interfacial Free Energy of Solid on Solid *fcc* Cu/*fcc* Pb Interface: A Molecular Dynamics Study

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Abstract. We have used classical molecular dynamics simulations to compute the solid on solid interfacial energy of Cu(001)/Pb(001) and Cu(111)/Pb(111) interfaces. Interfacial energy is difficult to obtain via experiments and different theoretical methods have been applied in published literature to estimate it. However, a majority of these theoretical calculations with either ab-initio or classical simulations report the interfacial energy only at 0 K although experiments are performed on alloy interfaces at finite temperatures. In this paper, we present a simple methodology to obtain the interfacial energy at any finite temperature of interest. We have applied it to calculate the interfacial energy of two Cu/Pb interfaces at 583 K (310 ^oC) for which experimental results are available. Our calculated finite temperature interfacial energy although underestimated is in much better agreement with the experimental values.

f0019

Ultra-Broadband Resistive Microwave Meta Absorber for Stealth Technology

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Abstract. This work demonstrates a novel ultra-broadband microwave metamaterial absorber that consists of an FSS resistive pattern that is made of 280 Ω/□ resistive ink imprinted on an FR4 dielectric interlayer with $0.029\lambda_L$ thickness.

The complete design was grounded with the help of a conducting copper plate. Simulation results revealed that a -10 dB reflection loss is found from 4-24 GHz with a high resonance peak of 17.9 GHz. Moreover, at resonance frequency, maximum reflection loss -29.9dB was achieved. The proposed absorber is angularly stable for 0^0-50^0 and polarization insensitive for 0^0-90^0. The absorber is well-suited for various X-band applications including communication devices, radar systems, and stealth technologies. Research suggests that the proposed metamaterial absorber is a feasible option for reducing electromagnetic waves in the X-band due to its compact size and exceptional performance.

f0020

Effect of Post Deposition Annealing Temperature and Duration on Structure of DC Sputtered Sn Films

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We report the systematic study on the growth and characterization of SnO_2 thin films deposited using DC sputtering method. The quality of the deposited film is governed by the choice of different process parameters that includes sputtering power, deposition pressure, substrate, substrate temperature, deposition duration, post deposition annealing temperature and duration, carrier gas etc. To realize polycrystalline thin films of SnO_2 from Sn targets, the post deposition temperature and duration is found to play the important role. Accordingly, in the present work SnO2 films deposited using Sn target, 25 W power, base vacuum of 2 x 10^{-5} mbar, substrate (glass) temperature of 100°C, deposition time of 15 min were investigated in detail to find the optimum post deposition annealing temperature and duration. XRD results indicate that the post deposition annealing temperature of 450°C and duration of 2 h resulted in the formation of polycrystalline SnO_2 films.

f0021

Deposition of Diamond –Like Carbon on Stainless Steel Substrate by RF Plasma CVD

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The DLC films are usually composed by a mixture of sp^2 and sp^3 hybridized carbon atoms, where thesp^3 and sp^2 ratio has a great influence on the characteristics of the film. As this ratio increases the properties of the film approach those of diamond; on the other hand, as this ratio decreases the film is considered more graphitic. As it would be expected, most of the techniques aim to characterize the type of amorphous and the amount carbon in the film, as well as the chemical composition of the whole structure composed normally by material matrix, interlayer and the doped DLC film, i.e. containing other elements to improve the properties. This means that the same DLC film could have totally different behaviours when tested in dry nitrogen atmosphere or moist air. We have used capacitively coupled RF plasma CVD technique to deposit DLC-SiO_2 films with varying of RF self bias (-250V to -550V). It is well understood that, change in RF self bias helps in controlling properties of deposited films namely, hardness, adhesion, optical properties etc. During Raman analysis, we have witnessed a trend in the peak-shift and I_D/I_G ratio of these deposited films which is reported in this work.

f0022

Study of Room Temperature Deposited Re-N Thin Films

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Rhenium (Re) placed in the middle of 5d transition metal series, is a well-known hard metal and it is predicted that the hardness of Re-N thin films will be even higher. But the high formation enthalpy of Re-N makes it challenging to synthesize its mononitride phase i.e. ReN. In this work, we present a systematic study on Re-N thin films grown at room temperature (300 K) using a reactive magnetron sputtering. The partial N_2 gas flow (RN_2) was systematically varied at 0, 5, 20, 40, 50, 60, 80, and 100% and changes in the deposition rate, structure and hardness were studied using x-ray reflectivity, x-ray diffraction and nanoindentation. As expected, Re is formed in a hcp structure at RN_2 = 0%, and up to RN_2 = 20% the parent Re phase is retained. Between RN_2 = 40 and 50%, a mixed phase of interstitial

Re(N) with ReN is obtained. At RN_2 = 60%, nanocrystalline ReN phase could be observed and beyond it gets disordered due to an oversaturation effect. It was observed that the hardness of Re-N phase formed with RN_2 = 20% was around 18.4 GPa whereas at RN_2 = 60% it was 13.3GPa with a standard deviation of 1GPa. These values are significantly higher as compared to pure Re thin films. It can be anticipated that further optimization of the deposition conditions would result in a fully stoichiometric, well-crystalline ReN phase with even higher hardness.

f0023

Structural and Optical Properties of NiO Thin Films Deposited Using Ni Pellet by PLD Technique with Varying Laser Energy

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In this work, NiO thin films were deposited by ablation of Ni pellet using a pulsed laser deposition technique with varying laser energy. The polycrystalline nature of deposited thin films are confirmed by the X-ray diffraction technique, and the transmittance is approximately 60 – 80 % in the visible region. The Band gap of the films is 3.45 – 3.62 eV, and the extinction coefficient shows good and approximate constant transparency in the visible region and higher absorption in the UV – region.

f0026

Bi_2Se_3 Nanorods on 2D $PtSe_2$ Decorated Pyramid Si Nanostructures for Optoelectronics Applications

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Two-dimensional (2D) and topological insulator (TIs) materials have been the focus of much research due to their significant physical, electrical, and optical properties, which could significantly contribute to the desire to integrate these materials with silicon (Si) technology directly. Among these 2D and TI materials, $PtSe_2$ and Bi_2Se_3 are highly desirable for various optoelectronics applications. Here, we report the growth of Bi_2Se_3 nanoplatelets and nanorods on 2D $PtSe_2$ decorated pyramid Si. The surface morphology of $Bi_2Se_3/PtSe_2$ heterojunction shows the formation of nanorods and stadium-shaped nanostructures with lateral size of 200-350 nm whereas $PtSe_2$ was found to be fully wrapping of pyramid Si nanostructures. Raman spectroscopy analysis revealed the formation of 2D $PtSe_2$ and rhombohedral Bi_2Se_3 structure. Further, photodetector characteristics in near-infrared regions will be investigated on these nanostructures.

f0027

Role of defects on 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 studied the role of defects on the structural, superconducting and plasmonic properties of ZrN thin film grown using a reactive nitrogen sputtering. A well-crystalline 200 nm thick ZrN film was grown at 723 K. XRD measurements confirmed that the lattice parameter of ZrN film comes out to be 4.55 Å, matching well with the theoretically predicted value. We performed Raman spectroscopy, low temperature electrical resistivity and variable angle spectroscopic ellipsometry (VASE) measurements in ZrN film. From Raman spectroscopy measurements it was observed that the points defects give rise to first order optical and acoustic modes that result in suppression of superconducting transition temperature down to 3 K as opposed to ≈7 K expected in polycrystalline ZrN films. VASE measurements confirmed that plasmonic response of ZrN film was not only significantly superior

than pure Zr but was found to be comparable to that of noble metals. Obtained results are presented and discussed in this work.

f0028

Improvement of film thickness uniformity on large area plano-concave substrate using inline magnetron sputtering technique for neutron and hard X-ray space astronomy application

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In neutron scattering experiment and hard X-ray space telescopes neutron and X-ray beams can be focused very efficiently by using supermirror on curved surface. Deposition of multilayer films on curved surface is challenging. Profile of thickness distribution for flat and concave surface have been simulated and explained for different target to substrate distance using the geometric formulation of sputtering. Using in-house developed rectangular cathode magnetron sputtering system single layer Ti films are deposited on flat surface and concave surfaces. In both the simulation and experiment lowest value of thickness non-uniformity (i.e ~4%) found in concave surface with higher substrate to target distance. Further, simulation of the optical performance of X-ray and neutron supermirror confirms 5% non-uniformity is acceptable for focusing.

f0029

Electrical and electrochromic studies on tungsten trioxide thin films

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Abstract. Tungsten trioxide (WO_3) thin films are grown by Electron beam evaporation under the oxygen partial pressure of $2x10^{-4}$ mbar at various substrate temperatures (T_s) varying from room temperature to 450 ^oC. The impact of substrate temperature on the electrical and electrochromic properties is reported. The room temperature electrical conductivity is noticed to be increased with substrate temperature. The highest coloration efficiency was found in the films deposited at Ts = 350 ^oC.

Keywords. Thin films of WO_3, EBE technique, Morphological, Electrical and Electrochromic studies.

f0030

Role of Dopants on Structural Stability of Iron Nitride Thin Films with Nominal Composition of α''-$Fe_{16}N_2$

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α''-$Fe_{16}N_2$ is known for having high saturation magnetization, yet establishing it for permanent magnet applications is difficult due to poor thermal stability and low magnetic anisotropy. Recent theoretical reports suggested that alloying α''-$Fe_{16}N_2$ with Cu, Mn, or Al could improve its thermal stability and magnetic anisotropy. To investigate these predictions, we deposited the thin films of undoped, 5 at. % Al, Cu, and Mn-doped films with a nominal structure: Cr(20 nm)/ [Fe-M-N (15 nm)/^{57}Fe-M-N (5 nm)]$_{\times 10}$/Al (2 nm) [M = 0, Al, Cu, Mn] by a dc magnetron sputtering. These samples were annealed at different temperatures for different periods. Further, x-ray diffraction (XRD) measurements were performed on the pristine and annealed samples to study phase formation and stability. The XRD patterns reveal that all pristine samples are amorphous and upon annealing, they crystallize into mixture of α-Fe, γ'-Fe_4N, and α''-$Fe_{16}N_2$. With Cu and Mn doping the crystallization behavior was analogues to undoped samples, but Al doping yielded a completely different behavior. Obtained results are explained in terms of influence of dopants on the diffusion process.

f0031

Self-Powered Environmental Monitoring via Polymer Photovoltaics

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This study investigates self-powered gas sensors based on inverted polymer solar cells (PSCs) with the structure ITO/ZnO/PBDBT/MoO_3/Ag. The PSCs of area 4 mm^2 achieve a photon conversion efficiency (PCE) of 12% which is among the highest reported photovoltaic performance for same device feature. For gas sensing, large-area cells (7 ± 0.5 cm^2) devices with a 3% PCE and an open circuit voltage (V_{oc}) of 0.75 V were used exhibiting a 13% sensitivity to NO_2. The sensitivity was measured by changes in V_{oc} under 10 W white LED illumination. Notably, V_{oc} returns to its original value after NO_2 removal. These results highlight the potential of polymer solar cells for self-powered gas sensor applications.

f0032

Low interface trap states in Solution Processed Silicon-Graphene oxide stacked MOS Device

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Graphene Oxide (GO) is a promising material for next-generation electronic devices. GO's exceptional electrical, mechanical, and thermal properties, along with its ability to form stable, low-leakage films at low processing temperatures, make it a strong candidate for enhancing device performance and scalability. This study explores the interface characteristics of GO in metal-oxide-semiconductor (MOS) structures, revealing low interface trap densities (D_{it}),) of 5.3×10^{11} $cm^{-2}eV^{-1}$ at 500 kHz and 7.3×10^{11} $cm^{-2}eV^{-1}$ at 1 MHz, comparable to high-quality SiO_2 dielectrics. The leakage current density of GO in metal-oxide-semiconductor (MOS) structures is 12×10^{-9} $A.cm^{-2}$ at 1 V. The low interface states are highly essential towards integrating GO for commercial device applications.

f0034

Structural and Optical Properties of NiO and $Ni_{0.75}Cu_{0.25}O$ and their Band Alignment at GaN Heterojunctions

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Epitaxial layers of NiO and $Ni_{0.75}Cu_{0.25}O$ were deposited on Al_2O_3(0001) substrates at different temperatures using RF magnetron sputtering. The out-of-plane and in-plane epitaxial relationships of the layers with respect to Al_2O_3 have been determined by X-ray Diffraction measurements which are: $[111]_{\text{layer}} \parallel [0001]_{Al_2O_3}$ and $[\bar{1}10]_{\text{layer}} \parallel [\bar{1}2\bar{1}0]_{Al_2O_3}$, respectively. The layers are found to have a two domain structure. With increasing growth temperature, the crystalline quality of the layers improves, the out-of-plane lattice parameters decrease and the optical band gaps increase. Cu substitution introduces a defect state within the NiO gap, along with a small reduction of the optical band gap. At the optimized growth temperature (750°C), the layers were deposited on GaN templates. Their crystalline quality and the epitaxial relationship with the GaN template were investigated. Band alignment properties at NiO ($Ni_{0.75}Cu_{0.25}O$)/GaN heterojunctions (HJs) were studied by photoelectron spectroscopy, showing Type-II band alignment at the HJs. The valence band offset (DE_V^{NiO}= ~1.2 eV, $DE_V^{Ni0.75Cu0.25O}$= ~1.4 eV) and conduction band offset (DE_C^{NiO}= ~1.5 eV, $DE_C^{Ni0.75Cu0.25O}$ = ~1.5 eV) at the HJs can be used in optoelectronic devices.

f0035

Theoretical Insights Towards Interfacial Engineering And Device Optimization Of $CH_3NH_3SnI_3$ Perovskite Solar Cells By SCAPS-1D

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Abstract: Perovskite solar cells (PSCs) have the potential to revolutionize the solar energy landscape with their high efficiency and low production costs, positioning them as leading candidates for next generation solar technology. However, their effective sustainable utilization is hindered due to major challenges viz. use of toxic Lead and rapid degradation issues. Addressing these obstacles is crucial to unlocking the full potential of PSCs and ensuring their practical widespread use. In line with this aim, the present study explores the significance of interfacial engineering in Lead free PSCs by introducing graphene interlayer which typically promotes hole extraction and reduces hole recombination. The Lead free, Tin based PSCs having device configurations as FTO/SnO_2/$MASnI_3$/Cu_2O/Au and FTO/SnO_2/$MASnI_3$/Graphene/Cu_2O/Au have been simulated by using SCAPS-1D program. The presented research

highlights the impacts of absorber layer thickness and total defect density (N_t) on performancce of Sn based PSCs. The optimized device, with power conversion efficiency (PCE) of 22.42%, is surpassed by the graphene modified optimized device, which achieved PCE of 25.06%. These results pave the way for developing cost effective, high efficiency PSCs.

f0036

Synthesis of Tungsten Carbide Thin Film by Ion Beam Sputtering

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Abstract: Thin films of tungsten carbide (WC) have been deposited on single crystal silicon wafers by Ion Beam Sputtering (IBS) technique using WC target. The effect of ion beam energies in the range of 800-1200 eV on the structure and morphology of thin films were investigated using X-ray reflectivity (XRR) and grazing incidence X-ray diffraction (GIXRD) techniques. It is observed that roughness of film decreases with increasing the ion beam energy up to 1000 eV. With further increase of energy, the roughness increases. At the optimum beam energy of 1000 eV, the minimum roughness of WC film, of ~2.5 Å is achieved with mass density of 14.50 g/cc (93% of bulk density), required for x-ray optics application. The observed variations of structure and morphology of WC film with ion beam energy have been discussed.

f0038

Resistive Switching in Epitaxial $La_{0.67}Sr_{0.33}MnO_3$/$SrMnO_3$/ $La_{0.67}Sr_{0.33}MnO_3$ Trilayer: Role of Lattice Strain

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In this study, we investigate the structural properties and current-voltage (I-V) characteristics of an epitaxial multilayer composed of $La_{0.67}Sr_{0.33}MnO_3$ (25 nm)/$SrMnO_3$ (70 nm)/$La_{0.67}Sr_{0.33}MnO_3$ (25 nm), grown on different substrates such as, $SrTiO_3$(100), $LaAlO_3$(100), Si (100) to tune the lattice strain. The current-voltage (I–V) measurements reveal distinct electrical behaviors depending on the substrate. The film grown on Si (100) exhibits notable resistive switching (RS) behavior, with a resistance ratio around 10 between the high resistance state (HRS) and low resistance state (LRS). Conversely, the $SrTiO_3$(100) and $LaAlO_3$(100) based films do not show RS but demonstrates a nonlinear I-V at lower voltages. While the observed I-V behavior is sensitive to substrate induced lattice strain, the present results have potential applications in future non-volatile based memory systems.

f0039

Influence of Tin doping on the Structure, Optical and Electrical properties of *c*-axis oriented Zinc Oxide films

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Abstract. In this study, Sn doped ZnO thin films with varying Sn dopant concentrations (0.5 %, 1 % and 1.5 %) were successfully fabricated on glass substrates with thickness 300 ± 10 nm by spin-coating method. The effects of dopant concentrations on the structural, optical and electrical properties of these films were investigated. All Sn doped ZnO (ZTO) films are found to grow in a hexagonal wurtzite crystal structure with strong (002) orientation of the crystallites, with no indication of metallic Zn, and Sn. A gradual decrease in the (002) intensity with increase in Sn doping is also observed. For all the ZTO thin films the average transmittance in the visible range was found to be ~ 90 %. From the transmission and reflection measurements the band gap energies were calculated, which exhibited nearly ~ 3.22 eV. The fabricated films exhibit n-type conductivity, as indicated by the Hall effect measurements with the lowest resistivity ($3.5 \times 10^{-1}\ \Omega\,\mathrm{cm}$) and highest mobility at room temperature for the 1.0 % Sn-doped ZnO thin film suggesting them as a potential candidate as transparent conducting oxide for optoelectronic applications.

f0040

Fabrication And Characterization Of Thin Film Coating On Large Area For Development Of X-ray Mirrors

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Development of mirrors for hard x-ray micro/nano focusing, requires large size optical coating with length of the order 300 mm on figured surfaces. To fabricate such mirrors, an ultra-high vacuum ion-assisted electron beam evaporation system is indigenously developed with an automated substrate rotation facility. Small-sized (20 mm × 20 mm) dummy Si substrates were placed at different locations over the area of ~ 300 × 100 mm^2 to analyze the structure and thickness uniformity of the coating. The process parameters were systematically varied to tailor the surface roughness, film density and uniformity of coating. Nickel thin films (average thickness ~42.5 nm) deposited at the optimized deposition parameters has a maximum thickness non-uniformity of ~4.4 %, with mass density ~99% of bulk value and average roughness ~1.2 nm. The calculated maximum slope error due to thickness non-uniformity is ~37 nano radian.

f0041

WS_2-Ag Nanocomposite-based SERS Substrates with an Ultralow Detection Limit for Pesticide Thiram

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Two-dimensional transition materials dichalcogenides (TMDCs) have a distinct advantage as a surface-enhanced Raman scattering (SERS) substrate because of their exceptional optical features, which facilitate efficient charge transfer with probe molecules and improve chemical enhancement. In this work, vertically oriented WS_2 flakes are synthesized on a Silicon (Si) substrate using the pulsed laser deposition (PLD) technique. The synthesized WS_2 flakes were decorated with Ag nanoparticles (NPs) using the thermal evaporation technique. The WS_2-Ag composite sample was characterized by FESEM, Raman and XRD. The composite of WS_2-Ag is investigated as a potential SERS substrate for detection of harmful pesticide thiram. Thiram is a common pesticide used as animal repellant in agricultural industry with many harmful effects on human health. Thiram is known to be highly toxic and life threatening to aquatic life. The WS_2-Ag composite SERS substrate effectively detects the toxic thiram up to the 10^{-13} M concentration.

f0042

120 MeV Au+ Irradiation Effects in [Gd/Fe]x10 Multilayers

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The present work explores the magnetic and structural behavior of Gd/Fe multilayers subjected to swift heavy ion irradiation. The GIXRD patterns indicate the broadening of the diffraction peaks of iron with increasing fluence. The analysis of XRR patterns indicate the significant increase in intermixed FeGd layer at the interface due to diffusion of the corresponding element at highest fluence (5E13 ions/cm2) irradiation in the studied multilayer. Variation of LMOKE loop with irradiation such as complete disappearance of DHL (double hysteresis loop) and development of the biasing field in the same 5E13 system etc. is discussed and it is attempted to explain the results in terms of intermixing with irradiation.

f0043

Stability Correlation and Bit Estimation of Aluminium Oxide Phosphate RRAM

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Resistive Random-Access Memory, RRAMs have emerged as promising solution by virtue of its analog nature and low-energy consumption. The stability analysis of RRAM is highly essential to gain deeper insights for practical applications. We explore Aluminium Oxide Phosphate (ALPO) – RRAM devices with fast-switching (50 ns) and significant non-linearity (0.54) for stability. The number of stable states that the RRAM could hold during long-term potentiation (LTP) and long-term depression (LTD) increases the computing efficiency and also lower the energy consumption during digital to analog conversions (DAC) and analog to digital conversions (ADC) as well. We also explore the correlation of the stability of the resistance-states with respect to cycles of program and erase. The stability of the resistance states with respect to time has been correlated further. The stability of the intermediate resistance states during LTP and LTD is also explored to estimate the number of bits that could be utilized using a single ALPO-RRAM device.

f0044

Assessment Of Load-Independent Hardness On Nonlinear Optical Sulphamic Acid Crystal

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The Indentation Size Effect (ISE) pertains to the correlation between a material's microhardness and the applied load in the low-load region. Estimated hardness values on nonlinear optical (100), (011), (0 $\bar{1}$ $\bar{1}$), (01 $\bar{1}$), and (0 $\bar{1}$ 1) faces of sulphamic acid (SA) crystal. All five different faces investigated exhibit reverse ISE. To comprehensively understand this ISE behavior in this crystal, employed several theoretical models. Each model defines a relationship between the applied load and the indentation size. Using the load-independent constants, the hardness values for the crystal under investigation were calculated without regard to load. Furthermore, the associated coefficient of correlation (CC) was found using the theoretical models for the best-fit data for the crystal.

f0046

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 anchoring mechanism of organic molecules on substrate surface. Herein, we report on the effect of annealing on the tilt angle of FePc molecules on Si (111) substrate surface. The tilt angle of FePc molecules was determined by measuring the XAS data at N K-edge at various angles of incidence of plane polarized synchrotron beam. Room temperature deposition of FePc on Si substrate resulted in amorphous thin films with randomly oriented FePc molecules. However, annealing of these amorphous films at 200°C led to highly ordered FePc molecules that followed edge-on stacking on Si substrate surface with an azimuthally averaged tilt angle of 75±5° between molecular plane and substrate surface.

f0048

SERS Activity of Hierarchical ZnO/Au Nanostructures for Trace Detection of Hazardous Dyes

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Abstract: In this paper, we have successfully prepared colloidal solutions of gold nanoparticles (0D) with a diameter <20 nm and nanorods (1D) bearing a high aspect ratio of 6.8, possessing tunable LSPR bands in visible and NIR regions, respectively. Further, unique nanosheet assembled 3D ZnO microflowers were prepared by a simple co-precipitation method, which is both cost-effective and easy to produce on a large scale. Herein, we investigated the effect of the dimension of gold nanostructures on the in-situ synthesized ZnO/Au hybrids for SERS application. SERS performance was evaluated by detecting a low concentration of Methyl Blue dye. All the samples having metal components depict excellent enhancement in the Raman signals of the dye, with ZnO-MF/AuNPs outperforming others.

f0049

Surface studies of Non-evaporable Getter thin film

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In order to achieve extreme high vacuum (XHV), non-evaporable getter (NEG) deposited by Magnetron sputter deposited thin film nowadays is considered as a suitable candidate. Its application in achieving XHV in various applications and instruments like vacuum pipe, particle accelerator, large Synchrotron Sources make them the most promising option as vacuum pump. In the present article, the authors report the Zr,Ti,V thin film deposition and behavior at different activation temperature. In addition, XPS characterization were performed to explore the change in elemental composition of the film surface.

f0050

Comparative Study of Structural and Morphological Properties Of ZrO_2 Thin Films Deposited in Normal and Glancing Angle Deposition Configuration

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In present work, structural and morphological properties of normally and glancing angle deposited (GLAD) ZrO_2 thin films deposited by RF magnetron sputtering have been investigated and compared. Both GLAD and normally deposited ZrO2 films exhibit preferential structural growth of monoclinic phase oriented in different directions. GLAD films also depict a tetragonal peak, which has been attributed to the presence of fine nano-crystallite size (~13 nm). RMS roughness values for GLAD and normally deposited ZrO_2 films are 5 and 1 nm, respectively. Dominant atomic shadowing is responsible for the high roughness of GLAD thin film.

g) COMPUTATIONAL METHODS, AND ELECTRONIC STRUCTURES

g0001

Molecular Engineering and Investigation of Novel Donor Molecule Based on [D-π-D] Type Architecture

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The Density functional theory (DFT) calculations have been performed on [D-π-D] type molecular structural model for designing the efficient donor moiety for dye sensitized solar cell application. The dye sensitized solar cell designed by Gratzel et al., in 1991 with ruthenium complex photosensitizer opened the new way of designing the organic solar cells. For this purpose, here in the paper, one novel donor molecule is designed and modelled on Gauss view interface. The designed molecule is named [Triphenylamine-Thiophene-Fluorene] as molecular system M1. The designed molecule was optimized under the framework of density functional theory using B3LYP hybrid functional and 6-31G(d,p) basis set level on GAUSSIAN 16W Software package. Further, the important electronic and chemical parameters like HOMO-LUMO energy gap, ionization potential, electron affinity are calculated. The excited state properties like absorption spectra, oscillator strength and excited state energy of the transition are calculated by utilizing the time dependent density functional theory along with CAM-B3LYP functional at same basis set level. The highest absorption maxima for the designed molecular complex was observed at 337.28 nm and open circuit voltage was reported to be 2.72 eV. From these photovoltaic calculation results, it is confirmed that the designed molecular complex which is based on D-π-D structure will be suitable for DSSC application.

g0002

A Computational Quest for Intermolecular Insights of Single Crystal Structure: A DFT and QTAIM Analyses

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The current study presents a comprehensive intermolecular interaction investigations for a novel single crystal using computational approach. The single crystal structure of a 3,3'-azanediylbis(5,5-dimethylcyclohex-2-en-1-one) (KSM) was confirmed via single crystal X-ray diffraction, revealing monoclinc crystal system with $P2_1/n$ space group and its unit cell parameters, respectively. The stability of the crystal architecture is attributed through short contacts and hydrogen bond interactions. Hirshfeld surface analysis is conducted to assess various intermolecular interactions based on the anisotropy of the topology. Additionally, Frontier Molecular Orbital (FMO) analysis and Molecular Electrostatic Potential (MEP) plots were utilized to explore the electronic structure and its physiochemical properties employing Density Functional Theory (DFT). Further, the study revolves around the Quantum Theory of Atoms in Molecule (QTAIM) and Non-Covalent Interactions (NCI) analysis along with ELF and LOL via multiwave function provide insights into the topology parameters. The integration of all these provides a detailed understanding to guide future research in the field of biophysics and material science.

g0003

DFT Investigation of Photocatalytic Properties of 2D WXY (XY= S, Se)/AlN vdW Heterostructure

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Photocatalytic properties of WXY (XY= S, Se)/AlN Heterostructure (HS) have been studied using Density Functional Theory. The WXY with AlN monolayer prefers an AA-stacking arrangement. The HSs are semi-conducting in nature with a band gap of 2.23eV -2.27eV. The band alignment of HSs is indirect type II behavior in which the valence band maximum is contributed by WXY (XY= S, Se) lies at K point, and the conduction band minimum is dominated by AlN monolayers lies between K-Γ point. The band edge diagram satisfies the minimum condition for water water-splitting redox reaction. Therefore, the results suggest that WXY (XY= S, Se)/AlN HSs are promising candidates for photocatalytic applications.

g0004

***Ab initio* study of intermediate band solar cell material: V substituted $MgSnP_2$**

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Intermediate band semiconducting materials have potential to use in high efficiency solar cell devices. Herein, we studied the optoelectronic properties of pure and V substituted $MgSnP_2$ using first principle density functional theory calculations. From our calculations, we found that $MgSnP_2$ is a direct band gap material with band gap value of 1.17 eV and V substitution creates intermediate band. Moreover, optical absorption spectra reveal that V substitution increase optical absorption at visible range compared with that of $MgSnP_2$ and silicon. Thus, it is understood that $MgSn_{0.94}V_{0.06}P_2$ belongs to the class of intermediate band solar cell material have potential to use in intermediate band solar cells.

g0005
Molecular Dynamics Study of Dental Material TEGDMA with 1% Gold Nanoparticles.
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We have conducted a molecular dynamic study on TEGDMA with 1% gold (Au) nanoparticles. Physical parameters such as lattice energy, heat capacity, zero-point energy, self-energy, dipole moment, and elastic constants were determined. Phonon density of states are compared with pure TEGDMA. Additionally, IR spectra were simulated and contrasted with those of pure TEGDMA. Significant differences were observed between these two materials, and an effort has been made to interpret these differences in terms of the nature of interactions in this research work.

g0006
Thermal Properties of BaS
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Using the ab-initio LCAO technique developed within the framework of density functional theory, the thermal properties of BaS are calculated. The total energy calculations are linked with the Birch-Murnaghan equation of state to find the structural properties of the ground state of BaS. To determine thermal properties such as thermal expansion coefficient, heat capacity, Grüneisen parameter and Debye temperature, the ab-initio calculations are coupled with the second generation package Gibbs2. The Debye Slater and Debye Grüneisen models are considered. The results are in agreement with some available theoretical results.

g0007
Electronic Structure And Thermoelectric Properties Of Single-layer 1D And 2D MoS2
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We have studied the structural, electronic, and thermoelectric (TE) properties of monolayer (ML) MoS2 in 1-dimensional (1D) and 2-dimensional (2D) structures using first-principles method based on density functional theory and followed by semi-classical Boltzmann transport theory. The monolayer 2D MoS2 exhibits a band gap of 1.66 eV, whereas the 1D MoS2 is metallic. The transport proper- ties such as the Seebeck coefficient, thermal conductivity, electrical conductivity, power factor (P.F.), and thermoelectric figure of merit (ZT) of ML 1D/2D MoS2 were computed at temperatures 300 K and 800 K. The 2D MoS2 is found to be more suitable for thermoelectric applications than 1D MoS2.

g0009
Intertwined Rashba Effect and Non-trivial Topology in Group I-IV-V based Non-centrosymmetric Compounds
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The exploration of coexistance of two distinct quantum phenomena within a single material enables the study of physics associated with relativistic electrons in solids. These compounds are knows as composite quantum compounds (CQCs). In present study, we predicted XGeBi and XSnM (X = K, Rb, Cs; M = As, Sb) compounds using density functional theory. Among which, XGeBi coined as intrinsic CQCs with topological insulating phase and giant Rashba splitting. The dynamical, mechanical and thermal stability is confirmed from phonon dispersion curves, elastic constants and AIMD simulations, respectively. The CsGeBi gives giant Rashba splitting energy of 153 meV with Rashba coefficient (α_R) of 4.10 eV Å while RbSnSb have trivial nature with of α_R 5.29 eV Å. This value of α_R (CsGeBi) is significantly large with previously reported non-trivial bulk materials. The α_R can be further enhanced by alloying with lowering symmetry constraints. In this regard, $CsGeSb_{(1-x)}Bi_x$ alloy with x = 0.50 indicates the non-trivial topology and record high Rashba coefficient. These materials have applications in spin-dependent electronic functions. The recent synthesis of NaSnX (X = P and As) materials indicate the likelihood of experimental studies.

g0013
First-Principles Calculations of Positron Lifetimes of Vacancies and Vacancy-Solute Complexes in Vanadium Including Positron-Induced Forces
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Many first-principles investigations are there to compute positron lifetimes in Vanadium. Still, not many calculations with accurate self-consistent densities while accurately handling the forces acting on ions induced by the presence of positron have been performed. In this work, we have incorporated self-consistent TCDFT calculations for computing the positron lifetimes of fully relaxed vacancies and vacancy-solute (Ti/Cr) complexes in V using open-source code ABINIT. This has been performed within the PAW method using GGA-PBE correlation functional. Through the inequal shifts of any particular ion in the presence and absence of positron, we can infer the importance of positron-induced forces. An increase in positron lifetimes has been observed in the case of fully relaxed vacancies as compared to the unrelaxed ones. This can be attributed to the repulsive positron-induced forces, which lead to the effective increase of open volume of defects. This work also shows that the binding energy of the Ti-vacancy complex is positive and it shows inward movement during relaxation towards vacancy, which indicates that Ti has a strong attractive interaction with vacancy in vacancy-solute complexes.

g0014
Thermodynamic Properties of Small Aluminum Clusters
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Abstract. Deep neural network~(DNN) based deep potentials (DP) model have been used to compute the thermodynamic properties of small Aluminum clusters. We have computed heat capacity and melting temperatures of Al_{25}, Al_{33}, Al_{39}, and Al_{44} clusters using multiple histogram technique. Extensive molecular dynamical simulations at 24 different temperatures have been performed for each cluster. Obtained results have an accuracy very close to the density functional theory (DFT). Our results show excellent agreement with the experimentally reported melting temperatures and heat capacity curves for all the investigated clusters

g0016
Prediction Of Debye Temperature Of The Materials Using Four Basic Machine Learning Regression Models
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Debye temperature (T_D) is one of the significant property of the crystalline materials and its knowledge is of prime importance for applications. Machine Learning (ML) is extensively used nowadays to explore the thermal properties of materials. In the present study, we have constructed a dataset of 1357 records from the AFLOW library and used it to predict the T_D employing four basic ML models: (linear regression (LR), Bagged Trees Ensemble regression (BATER), Boosted Trees Ensemble regression (BOTER) and Support Vector Regression (SVR). The predicted accuracy in T_D in terms of R^2 and RMSE were 98.11% and 47.17, 97.73% and 51.74, 97.25% and 56.99, 97.68% and 52.35 for LR, BATER, BOTER, SVR respectively. The testing accuracy of all the four used ML models in terms of R^2 are better than the recently reported value of R^2 equal to 95.1% of the gradient boosting (GB) ML model with a dataset of 5412 records collected from the same AFLOW library. Further, LR is the best performing model among all the four used model in testing results in the present study and also compared to the best ever reported testing accuracy of R^2 = 95.1% and RMSE = 48.5 to the best of our knowledge. Moreover, this LR testing result is also better than R^2 = 97.8% for 42 records of monoclinic crystal.

g0017

Structural and Optoelectronic Properties of Monolayer $ScBiS_3$ under Pressure: A First Principle Approach

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The optoelectronic Properties of ScBiS3 monolayer have been investigated at different pressures up to 16GPa using a first principles calculations based on DFT. With the increasing pressure band gap of monolayer decreasing and at the 16GPa the band gap becomes zero and material turns into metal. By examine the optical properties of material at various pressure, we have been observed that at 16GPa material stat absorption from infrared region which make it suitable for the application in infrared optoelectronic devices and technology.

g0018

Tuning MXene Monolayer via -OH Functionalization: DFT Insights into Structural and Optoelectronic Properties

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The present study represents the effect of functional groups (-O and -OH) on the structural and optoelectronic properties of Y_2C and ScYC monolayers. Both Y_2C and ScYC monolayers have been functionalized with -O and -OH group to form Y_2CO_2, $Y_2C(OH)_2$, $ScYCO_2$, and $ScYC(OH)_2$ monolayers. Among all, except $ScYCO_2$, all the monolayers are kinetically stable confirmed by phonon dispersion relation. Y_2C monolayer with oxygen functionalization on both the surfaces (Y_2CO_2) shows insulating nature with indirect bandgap 3.67 eV, while Y_2C and ScYC monolayer with -OH functionalization ($Y_2C(OH)_2$ and $ScYC(OH)_2$) shows semiconducting nature with direct bandgap 1.12 eV and 1.09 eV, respectively. Optical properties suggest that -OH functionalized monolayers show absorption in visible as well as in IR regions. Overall findings suggest application of $Y_2C(OH)_2$ and $ScYC(OH)_2$ monolayers in optoelectronic devices.

g0019

Effect of Bi-axial Strain on Structural and Electronic Properties of 2D Sc_2CO_2 MXene

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Using Density Functional Theory, we have investigated the effect of biaxial strain on the structural and electronic properties of Sc_2CO_2 MXene. The calculations have been performed by applying a bi-axial strain of ±5%. The results show that the stability of Sc_2CO_2 increases with tensile train with maximum binding energy value at a tensile strain of 3%. The electronic properties show that Sc_2CO_2 is naturally semiconducting with a band gap of 2.01eV. When compressive strain is applied, the band gap increases to 2.06eV with 1 % strain which further decreases to 1.19eV whereas with tensile strain band gap decreases to 1.68eV with ±5% strain. The band alignment remains indirect up to 3% in which the valence band maximum lies at Γ point, and the conduction band minimum lies at K point. At 5%, there is a change in band alignment, and the monolayer becomes direct. The results suggest that the electronic

properties of Sc_2CO_2 can be tuned with strain for desired applications such as photocatalytic and optoelectronic devices.

g0020

Generation of IPG Glass Models and Study of Their Irradiation Characteristics: A Hybrid MC- MD approach

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This study investigates the radiation damage and structural properties of iron phosphate glass (IPG) using a hybrid MC-MD approach. Random configurations of IPG are generated with an in-house potential-free Monte Carlo method and subsequently melt-quenched using classical molecular dynamics simulations. This process creates highly randomized, amorphous structures. The radiation damage is then simulated in a cell containing about 80,000 atoms, with a primary knock-on atom (PKA) introduced at various energies and directions. The velocity-velocity autocorrelation function reveals that energy dissipation in the ballistic regime is independent of PKA energy. The study also shows minimal recombination of defects and highlights a higher number of oxygen point defects compared to other species. The peak number of defects increases linearly with PKA energy, consistent with NRT predictions.

g0022

A DFT study of electronic, optical and mechanical properties of $LiBaBr_3$ perovskite for opto-electronic applications

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We present ab initio calculations to determine the electronic, optical, and mechanical characteristics of $LiBaBr_3$ opto-electronic material. Opto-electronic simulations for lead-free perovskite compound are done using Perdew-Burke-Ernzerhof approach. The electronic band structure computations for $LiBaBr_3$ revealed a band gap of 2.895 eV with indirect nature. Moreover, the dielectric constant and absorption coefficient of $LiBaBr_3$ are reported that suggest its possible utilization in opto-electronic devices.

g0023

***Ab-initio* Study of Structural and Electronic Properties of $HoTe_3$ under High Pressure**

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Ab-initio calculations were carried out on $HoTe_3$, an ideal quasi 2-D layered material, to understand the effect of high pressure on its structural and electronic properties. In this investigation, we find that the ambient orthorhombic *Cmcm* phase of $HoTe_3$ remains stable up to 50 GPa. The calculations show that its compressibility is highly anisotropic with [010] being the most compressible axis. This anisotropy is a direct consequence of its layered structure. The calculated pressure-volume data is fitted using a third order BM equation of state which results in the bulk modulus, $K_0 = 45.08$ GPa and its pressure derivative, $K_0' = 4.72$. The electronic band structure calculations reveal that $HoTe_3$ is a metal with the major contributions from the Te-5*p* orbitals.

g0024

A DFT Study on Optoelectronic Properties of $GaAlS_2$ Homo-bilayer

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In the present study, the optoelectronic behaviour of $GaAlS_2$ homo-bilayer has been explored using a density functional approach. The calculation of adhesive energy and phonon validates the energetic and dynamic stabilities of the $GaAlS_2$ bilayer. The band gap of bilayer $GaAlS_2$ homo-bilayer is 2.30 eV which shows its indirect semiconductor

nature. The optical behaviour indicates a significant enhancement in the absorption of the $GaAlS_2$ homo-bilayer compared to the $GaAlS_2$ monolayer. There is a significant increment observed in the reflectivity of the $GaAlS_2$ homo-bilayer. The outcomes suggest that $GaAlS_2$ homo-bilayer is a promising applicant for optoelectronic devices, UV detectors and UV absorbers.

g0025

MgClBr vdW homobilayer as a promising UV-light detector

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In this study, the optoelectronic characteristics of a newly predicted MgClBr homo-bilayer have been examined using Density Functional Theory. Two different stacking configurations, AA and AB are considered for the calculation. To confirm its thermal and dynamical stability, both AIMD simulations and phonon spectrum analysis have been conducted, demonstrating that it is stable in both aspects. The MgClBr HBL shows the insulator nature with wide bandgap of 5.91 eV, using HSE06 functional. Additionally, the absorption spectrum covers a broad range of spectrum. The obtained static refractive index is 1.42 for MgClBr HBL. However, there is a significant absorption in the UV region. This highlights its potential for use in opto-nano devices applications and UV-light detectors.

g0026

Studies of Structural and Electronic Properties of HfS3 and ZrS3 Under Pressure

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Abstract: Transition metal trichalcogenides are of current interest because of their various possible applications in battery, catalysis, photo-voltaic, thermoelectric devices etc. Using density functional theory based calculations we have studied structural and electronic properties of HfS3 and ZrS3 at ambient and high pressure conditions. Our results show that both HfS3 and ZrS3 undergoes isostructural phase transition near 16 and 18 GPa respectively. We found both the Satoms of the S-S dimer present in the structure are connected with same transition metal atom in low pressure phase but they are connected with different transition metal atom in the high pressure phase indicating changes of bonding between metal atom and S-S dimer.

g0028

Structural and Electronic Properties of Quaternary Heusler Alloy CoMnVAl: A First-Principles Study

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We study the electronic structure and topological properties of quaternary Heusler alloy CoMnVAl. We use a combination of both density functional theory (DFT) and tight binding approximation (TBA) to investigate its properties. Our study shows that CoMnVAl is a non-magnetic semimetal. A finite Berry curvature is present the system which gives rise to a small intrinsic anomalous Hall conductivity of 17 S/cm at the Fermi level.

g0029

Zircon to Scheelite Phase Transition in EuAsO4: First Principles Simulation

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Europium arsenate ($EuAsO_4$) crystallizes in the tetragonal zircon structure (space group $I4_1/amd$). Using density functional theory (DFT) simulations employing Quantum Espresso, we discovered a pressure-induced first-order structural phase transition to the scheelite structure (space group $I4_1/a$) around 3 GPa. This transition involves significant changes in unit cell parameters, bulk modulus, and polyhedral compressibility, providing new insights into the high-pressure behavior of this material.

g0030

Topological electronic structure and anomalous Hall effect in altermagnetic RuO_2

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Altermagnets are distinguished from antiferromagnets with a momentum-dependent spin-splitting and broken effective time-reversal symmetry. The broken time-reversal symmetry results in a nonzero Berry curvature field, resulting in a nontrivial topology and ferromagnet-like responses such as the anomalous Hall effect in altermagnets. Based on first-principles calculations and symmetry analysis, we show that RuO_2 is an ideal *d*-wave altermagnet with rich topological electronic states. In the absence of spin-orbit coupling, it supports Weyl nodal loops with drumhead surface states. With spin-orbit coupling, some nodal loops are gapped to realize Weyl fermions and Fermi arc surface states. Moreover, we show that the broken effective time-reversal symmetry in RuO_2 generates a Néel vector-dependent finite anomalous Hall conductivity. We also discuss the topological properties as a function of the strength of Coulomb repulsion in RuO_2.

g0031

Quantum Computation of Small Atomic Clusters Using Subspace-Search Variational Quantum Eigensolver

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The subspace-search variational quantum eigensolver (SSVQE) algorithm is used on various atomic clusters of Be, B and C atoms to find their ground state and 1st excited state energy values. Various approximations such as active space and freeze core have been used to reduce the quantum qubit in the computation. The approximations affect the energy values for quantum mechanically big clusters (C_4, B_4, etc.) This work also shows the use of the application of SingleExcitation and DoubleExcitation to build the ansatz. The final calculated energy values are compared with those calculated by the Hartree-Fock and DFT methods. The findings show that, when the ansatz and optimization are properly customized to the given situation, the SSVQE algorithm can consistently and accurately find both ground and excited state energies. This research highlights SSVQE's potential as a formidable tool for quantum simulations on upcoming quantum technology, providing a mechanism to achieve more accurate and thorough quantum chemistry and material science computations.

g0033

CdS-Janus van der Waals Heterostructure for Green Hydrogen Fuel Production

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Abstract. Photocatalysis is one of the promising methods to produce green hydrogen by splitting the water molecule under solar irradiation. There are a large number of studies available on the CdS based photocatalyst due to its unique photocatalytic properties. However, CdS in its pristine form has a drawback of photoinstability due to photocorrosion effect. To improve the performance of the pristine CdS, a 2D-2D van der Waals heterostructure has been constructed with the Janus monolayer In_2SeTe. Due to their structural asymmetry, Janus materials have some peculiar properties associated with them. The properties of the constructed heterostructure have been investigated using Density Functional Theory. The geometrical and electronic properties of the constructed heterostructure have been investigated systematically. The favorable type-II band edge alignment and the built-in electric field in the heterostructure are suggesting the CdS-In_2SeTe as an excellent photocatalyst for hydrogen production.

g0034

Study of Mechanical Properties of Nanowires (Ni, Cu, Ag) using Classical Molecular Dynamics Simulations

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This study investigates the mechanical properties of various nanowires using classical molecular dynamics simulation. This study mainly focuses on variation of diameter of various nanowires and to observe the size effect on stress strain curve. The primary aim is to obtain stress strain curve of various nanowires and observe their mechanical properties response during application of tensile stress. The result reveals that the mechanical properties of the nanowires are size dependent and it is significant varying with the size. The study provides an insight about various nanowires like nickel, copper and silver contributing to the understanding of nanomaterials for the application in various fields such as light sensors, gas sensors, resonators etc.

g0035

The Effect of Second-Neighbor Hopping on the Weyl points in the Antiferromagnetic Phase of Rashba-Hubbard Model

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We use Hartree-Fock meanfield theory to demonstrate the presence of Weyl points in the antiferromagnetic phase of t – t' Rashba-Hubbard model for a 2-D square lattice. Previously, the Weyl semimetallic state with antiferromagnetic order was obtained in the ground state phase diagram of Rashba-Hubbard model considering nearest neighbor hopping (t'), when the band was half filled. Even in the presence of second-neighbor hopping, the antiferromagnetic phase stabilizes, but only for weak Rashba spin-orbit coupling (λ). In the current work, we find that, immediately above a critical on site Coulomb interaction, the Rashba type spin-orbit coupling generates Weyl points in the band dispersion, which are shifted away from the Fermi-surface. To verify the obtained Weyl points, we calculate the Berry connection and winding numbers associated with them.

g0038

Mie-Grüneisen Equation of State of Li_2C_2 based on First Principles

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In the current study we employ Mie- Grüneisen form of thermal Equation of State (EOS) to determine pressure - volume-energy relationship of Li_2C_2 over a wide range of compression considering pressure-induced phase transition. Three distinct analytical forms of volume dependence of Grüneisen parameter, as proposed by Slater, Dugdale-MacDonald and Vashchenko-Zubarev, in conjunction with DFT-predicted cold EOS are utilized for this purpose. Our study reveals that, although pressure-dependent Grüneisen parameter differs significantly among the three models, it has a minimal impact on the EOS. Further, it is observed that ambient Grüneisen parameter predicted by Dugdale-MacDonald model closely aligns with the value obtained from first principle calculations.

g0039

Design and Performance of Novel Perovskite Solar Cell: FTO/SnS_2/$RbGeBr_3$/Au Configuration Explored via DFT, ML and SCAPS-1D Studies

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The present paper is aimed to predict the Solar cell performance of $RbGeBr_3$ perovskites from Density Functional Theory (DFT) study and Machine Learning (ML) models and validated through the Solar Cell Capacitance Simulator (SCAPS-1D). We first investigated a single-junction $RbGeBr_3$ perovskite solar cell, achieving a power conversion efficiency (PCE) of 18.25% from DFT calculations. Utilizing ML , we predicted solar parameters based on basic input features and material layers. A dataset containing 42,400 photovoltaic devices was utilized. After screening the required input properties, we used 4200 DFT-calculated data points of Perovskite Solar Cells from the MaterialsZone repository for training and validation. Among the algorithms, the Random Forest model achieved the best performance. For the validation we employed the Solar Cell Capacitance Simulator (SCAPS-1D) with an assumed configuration of Al/FTO/SnS_2/$RbGeBr_3$/Au. The input parameters for the SCAPS-1D software were determined, and

the ML-predicted values for FF, V_{oc}, J_{sc}, and PCE showed good agreement with SCAPS-predicted values, yielded the PCE of 33.8%. Therefore, the mentioned structure would be suitable for experimental studies to fabricate high-performance photovoltaic devices.

g0041

Point-Defect Induced Monolayer 2H-MoS_2 for Spintronics – A First Principles Study

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Identifying a new material with high spin polarization for spintronics applications is an emerging trend in current research perspectives. Two-dimensional materials have a wide range of applications such as optoelectronics, spintronics, and nanoelectronics. In this present investigation, we explored the electronic and magnetic properties of pristine and point defect-induced 2H-MoS_2 systems for spintronics applications. The electronic and magnetic properties of monolayer 2H-MoS_2 and point defect-induced 2H-MoS_2 were calculated using the Vienna Ab-initio Simulation Package (VASP). The calculations revealed that the defective MoS_2 has conducting behavior in spin up direction and semi-conducting behavior in spin down direction. The spin-polarized calculation was performed to analyze the magnetic properties of the point defect-induced 2H-MoS_2. The calculated total magnetic moment of the point defect-induced 2H-MoS_2 is 1.789 μB/cell. The spin-orbit coupling is also employed to confirm the metallic behavior in the spin-up direction. The study illustrates that the point defect-induced monolayer MoS_2 is experimentally favorable spintronic material that leads to technological advancement in the spintronics field.

g0042

Ab-initio simulations lead to Rubidium based lead-free perovskite photovoltaics

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Metal halide perovskites, characterized by their tunable bandgap and high optical absorption, are emerging as cost-effective alternatives to silicon in solar cells and other optoelectronics. This study explores lead-free RbBX3 perovskites (B=Sn, Ge; X=I, Br, Cl), revealing their potential for LED applications through DFT-based structural, electrical, and optical analyses. The findings highlight the ability to adjust the bandgap by substituting halogens, with Ge substitution offering the most promising absorption properties for solar cell use.

g0043

Structural, Electronic and Thermal Stability of Janus Silicene monolayers: First-Principles Study

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This study employs first-principles density functional theory to investigates the structural, electronic, and thermodynamic stability of Janus silicene monolayers functionalized with chlorine atoms on one side and hydrogen or lithium atoms on the other, referred to as Si_2HCl and Si_2LiCl, respectively. Our findings reveal that the presence of hydrogen and lithium atoms increases the Si-Si bond length compared to pristine silicene, indicating significant covalent bonding interactions. Electronic band structure and density of states analyses show that Si_2HCl has a direct band gap of 1.92 eV, making it suitable for optoelectronic applications, while Si_2LiCl exhibits a narrower band gap of 0.42 eV, advantageous for applications requiring higher electrical conductivity. Phonon dispersion calculations confirm the kinetic stability of these Janus structures, evidenced by the absence of imaginary phonon modes and high phonon frequencies.

g0044

Experimental And DFT Studies On Cubic Structured ε -FeSi Semiconductor

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In the present work we experimentally synthesized cubic structured FeSi using planetary ball mill. The structural and electrical properties were compared with DFT results. The obtained FeSi phase is confirmed using X-ray diffraction and electrical conductivity studies are conducted using Hall measurement of the sample at different temperatures. To gain deeper insights into the electronic structure of FeSi, computational method called density functional theory (DFT) calculations are conducted within generalized gradient approximation (GGA) framework using Quantum ESPRESSO software. Additionally, the density of states (DOS) and projected density of states (PDOS) of FeSi are carefully evaluated to understand the electronic distribution within the material. The obtained values of band gap and lattice parameter show consistency with previous works.

g0045

Investigation of native defects on the PbIBr Janus monolayer: A DFT study

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The growth of any material especially two-dimensional layers involves unavoidable defects. These point defects will have a significant effect on the geometry, electronic and optical properties of the structure. Herein, we investigate the influence of point defects on the electronic properties of the Janus monolayer PbIBr using first-principles based Density Functional Theory (DFT) calculations. The formation energy of the point defects I, Br and Pb in PbIBr has been calculated. Using the calculated formation energy, we found the concentration the three different defects as a function of temperature. Later, to understand the electronic properties of the defected structures we have calculated electronic density of states (DOS) and observed the evolution of the defect states in the band gap region.

g0046

Assessment of Fe-Zr Alloys as Host Matrices for High Level Nuclear Metallic 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.

g0048

First Principles Calculations on the Structural and Electronic Properties of Pt-Ir Alloys

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We investigated the impact of pseudopotential and Ir doping concentrations (ranging from 0% to 100%) on the geometric and electronic properties of PtIr alloys. Using ab initio quantum computations in the Material Studios program, we analyzed lattice constants, crystal structures, and total energy (E_{tot}) of unit cells. Electronic structures were validated through band gap (E^g), projected density of states (PDOS), and total density of states (TDOS). Our findings highlight the crucial role of pseudopotential and Ir doping concentration in shaping the physical characteristics of Pt-Ir alloys.

g0049

Investigating Cross Sections of Biologically Significant Molecules using Electron Impact Ionization

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The study of charged particle motion in the vicinity of a nucleus is one of the most significant collision processes in atomic and molecular physics. This study is useful not only in the fields of astrophysics, biology, and medicine but also in the development of various experimental and calculation methods. In the coincidence study, triple differential cross sections (TDCS) are obtained to provide detailed information about (e,2e) collision processes, which have been of interest since Ehrhardt's pioneering work. In recent years, many atomic and molecular targets like H_2, N_2, CO_2 and H_2O have been the subject of extensive ionization cross-section studies. The ionization cross-sections will be obtained in the first Born approximation formalism which will be extended to the next higher order i,e. the second Born approximation using orientation averaged molecular orbital (OAMO) approximation. The post-collision interaction (PCI) is also included to treat the interaction between two outgoing particles. The obtained results will be compared with the recently available measurements and analysed in terms of binary and recoil peak positions and intensities in different geometrical conditions.

g0051

DFT Analysis of Holmium-Doped Mg-ZnO Nanostructures: Structural, Electronic, and Magnetic Properties.

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This study investigates how doping ZnO with magnesium (Mg) and holmium (Ho) impacts its characteristic properties. Using Density Functional Theory (DFT), we analyzed a ZnO lattice with the composition $Zn_{17}Mg_2$ Ho_1 $O_{16.}$ Our findings reveal that Mg doping decreases ZnO's bandgap from 0.758 eV to 0.216 eV, increasing its electrical conductivity. Holmium doping shifts the Fermi level into the conduction band, enhances magnetic characteristics with spin-polarized 4f states, and improves photoconductivity. Additionally, Mg and Ho doping contributes to the stability of ZnO's hexagonal phase, with lattice parameters changing from a=3.250 Å to 3.254 Å for Mg doping and compressing to 3.065 Å for Ho doping. Holmium doping induces ferromagnetism in Mg-doped ZnO through increasing spin polarization and enhancing magnetic interactions in the 4f states.

g0052

A Review of Theoretical Approach to Study The Anomalous Behaviour of Strongly Correlated Heavy Fermion System

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Here we try to review our theoretical approach to study the anomalous behavior of heavy fermion system. As heavy fermion system shows low temperature anomalous behavior such as large effective mass, by lowering temperature decrease in electrical resistivity and non-dependence of magnetic susceptibility with temperature and linear dependence with temperature. Here considering the Periodic Anderson Model and using Zubarev technique for Double time temperature dependent Green function method we evaluate electron self- energy and spectral density. In order to explore the low temperature anomalies such as elastic constant, resistivity has been explored with long wavelength (q=0), finite 'q' and finite 'T'. Putting $\omega \rightarrow \omega+i\eta$, the electron self-energy evaluated with imaginary and real part which can be utilized to calculate the elastic constant and resistivity. f electron moment at low temperature interacts with each other and electron in the conduction band strongly resulting in a highly correlated electron state which shows the anomalies in heavy fermion systems. Therefore, we consider electron-phonon interaction in the system Hamiltonian and investigate its effect on elastic constant and resistivity. The impact of different system parameters including 'd' refers the location of f- level, 'r'- electron-phonon coupling strength and 'g'- the coupling constant on the anomalies has been inspected.

g0054

Structural, electronic, and magnetic properties of the ternary alloy Gd2Ru3Ge

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Density function theory calculations are performed using full potential linearized augmented plane wave (FP-LAPW) method within GGA formalisms to investigate the electronic properties of Gd2Ru2Ge alloy. Structural and magnetic properties of an intermetallic Gd_2Ru_3Ge compound have been investigated in this paper. Structure optimization studies

clearly shows that the ferromagnetic state is preferred over paramagnetic state. The compound shows a ferromagnetic metallic character.

g0056

Investing the mechanism of magnetic moment suppression in Quaternary Heusler Alloy CoCrVAl

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The alloy CoCrVAl (CCVA) has been investigated using the framework of density functional theory. Within *full potential linearized augmented plane wave* (FP-LAPW) method the pristine alloy shows ferrimagnetic ground state with total magnetic moment of ~1.0 bohr magneton, however a recent experimental study has found that there is no resultant magnetic moment in this alloy. To investigate the origin of such inconsistency, we have employed *coherent potential approximation* (CPA) based Korringa-Kohn-Rostoker method to investigate the energetics and magnetic properties of this alloy. Our results find that the intermixing of cobalt and chromium atoms in the crystal can suppress the magnetic moment yielding in zero resultant magnetism.

g0057

Superconducting State Parameter Of Actinide Based High Entropy Alloy

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Abstract: The superconductivity in actinide-based high entropy alloy Superconductor (AHEASC) $(TaNb)_{0.5}(TiZrHf)_{0.5}$ is studied in the framework of BCS theory and McMillan's formalism has been studied for the investigation of superconducting state (SC) parameters viz., Coulomb pseudopotential μ^*, electron–phonon coupling strength λ, SC transition temperature T_C, interaction strength N_0V, band gap Δ, energy or mass renormalization parameter Z_0 and isotope effect exponent δ. BCS theory in conjunction with McMillan's formalism has been used for the investigation.

g0058

Ab Initio Calculations On Superconducting, Electronic Properties Of $YLuHg_6$

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In this study, the first principle calculations using density functional theory within generalized gradient approximation were done for $YLuHg_6$, and its superconducting and electronic properties were calculated. The phonon dispersion curve shows that the compound is found to be dynamically stable. It is found to be superconducting with the electron-phonon coupling constant 0.67 and has a T_c of 3.311 K. Our results show that $YLuHg_6$ is a new entrant in the family of electron-phonon-mediated superconductivity.

g0060

Exploring Single and Double-Side Functionalization of Aluminum Nitride Nanotubes with Formic and Fumaric Acids for Drug Delivery: A DFT Study on Hydroxyurea Interaction

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Nanotechnology has revolutionized biomedical sciences, particularly in targeted drug delivery. This study investigates Aluminum Nitride Nanotubes (AlNNTs) functionalized with formic acid (FA) and fumaric acid (FUA) as drug carriers. Using density functional theory, functionalization enhances the interaction of AlNNTs with biological systems by increasing bond lengths, decreasing bond angles, and shifting towards sp^3 hybridization. These changes improve solubility and reduce toxicity. Bandgap analysis shows a significant reduction from 3.28 eV in pristine

AlNNTs to 1.18 eV for double-side functionalized systems. Additionally, functionalization boosts the intensity of valence band states and increases the dipole moment, indicating higher polarity. The ionic character of AlNNTs increases to 49% with double-side functionalization, and the Gibbs free energy of solvation indicates favorable conditions for functionalization, with fumaric acid enhancing solubility the most. Drug interaction studies reveal that double-side functionalized AlNNTs with fumaric acid strongly bind to hydroxyurea, with a binding energy of 0.7 eV. These results highlight the potential of fumaric acid-functionalized AlNNTs for effective drug delivery applications.

g0061

Density Functional Theory Analysis of Allicin and Resveratrol Interactions with Pristine and Glutamine-Functionalized Boron Nitride Nanotube

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The interaction of bioactive molecules such as allicin and Resveratrol with pristine (5,5) Boron Nitride Nanotube (BNNT) and functionalized BNNT with glutamine was investigated using Density Functional Theory (DFT). By examining the Interaction energies, structural parameters, and electrical properties, this study seeks to clarify the strength of interactions of these drugs with BNNT. The results reveal significant adsorption energies, indicating that the drugs and BNNT have persistent interactions. The electronic characteristics analysis indicated that the adsorption of these bioactive compounds onto BNNTs leads to notable changes in the electronic structure, including modifications in the band gap. This comprehensive theoretical insight underscores the viability of BNNTs as nanocarriers, offering a pathway for the development of enhanced drug delivery platforms.

h) DIELECTRIC, FERROELECTRIC AND PIEZOELECTRIC

h0004

Enhancement of Relaxor Properties in NKBT via BMN

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Perovskite solid solution of **(**1-x) $Na_{0.2}K_{0.3}Bi_{0.5}TiO_3$ -x $BiMg_{(2/3)}Nb_{(1/3)}O_3$ or (1-x) NKBT-x BMN were synthesized by solid-state reaction technique(referred to as (x=0) 0 BMN and (x=0.10)10 BMN. X-ray diffraction results confirm a pure perovskite structure for all samples studied. Surface morphology analysis demonstrates that grain size of the samples increases with BMN addition. Dielectric measurements reveal relaxor-like characteristics in the NKBT-BMN ceramics, with broadened phase transition peaks transitioning to temperature-stable permittivity as BMN content increases. The enhancement of the diffusive factor further supports these findings. This study provides a potential application of lead-free ceramics as a dielectric capacitor in the era of electronic technology.

h0005

Analysis of Structural, Optical, and Dielectric Properties of SiO2-Si Systems Under Mechanical Milling

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We performed mechanical alloying of Silicon dioxide (SiO_2), and a mixture of SiO_2 and silicon (Si) separately. The milled powders were heat treated at 1000 °C under vacuum to explore their structural, optical, and dielectric properties. X-ray diffraction patterns have indicated the single tetrahedral phase (P 32 2 1) in mechanically milled samples of SiO_2, whereas a mixture of hexagonal phase (F d 3 m) of Si and tetrahedral phase of SiO_2 were observed in mechanically milled samples of SiO_2 and Si. The structural parameters of the milled samples did not change significantly under post heat treatment of the samples. X-ray photoelectron spectroscopy indicated + 4 and + 2 charge states for Si ions in the mixed-phase sample. UV-Visible spectroscopy reveals the direct and in-direct optical bandgap in the range of 4.6 - 4.9 eV and 1.1 – 2.0 eV, respectively. The heat treatment of mechanically milled formed a material of low dielectric loss and dielectric constant in the range of 3-5.

h0006

Insight Into the Electrical Properties of Ni Doped $SrBi_2Nb_2O_9$ Aurivillius Ceramics Prepared Through Microwave Sintering Method

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The polycrystalline $Sr_{0.8}Ni_{0.2}Bi_{1.95}La_{0.05}Nb_2O_9$ (NSBN) ceramics were synthesized using a single-step microwave sintering method. Frequency dependent variation of electrical measurement demonstrates high dielectric constant and low dielectric low, irrespective of temperatures. AC conductivity study indicates the polaron-assisted conduction mechanism in prepared composition, which further obeys Jonscher power law. Complex impedance spectroscopy (CIS) techniques have been incorporated in the present work to examine the intra- and intergranular contributions to the impedance in NSBN ceramics.

h0007

FTIR and Raman spectroscopy of Nd doped calcium copper titanate Lead free ceramics

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The synthesis of pure and Neodymium-doped $CaCu_3Ti_4O_{12}$ ceramics was carried out using Solid State Reaction (SSR) technology. The pure calcium copper titanate (CCTO) sample went through a 10-hour calcination process at 1000°C, followed by fusion for 8 hours at 1050°C in a muffle furnace. To verify the distinct phase and crystallinity of the synthesized materials, X-ray diffraction (XRD) analysis was conducted. The precise selection of peak broadening parameters using the Debye-Scherer and Williamson-Hall methods significantly affects the measurement of crystallite size and strain. Fourier Transform Infrared (FTIR) spectra showed the presence of vibrational modes involving Ca-O,

Cu-O, and Ti-O-Ti bonds at specific wavenumbers: 606 cm^{-1}, 525 cm^{-1}, and 463 cm^{-1}, respectively. The Raman spectra of single crystals of CCTO were analyzed, revealing the presence of eight active phonon modes (2Ag + 2Eg + 4Fg) associated with the Im3 crystal phase. These findings provide additional information on the vibrational behavior of CCTO and contribute to our understanding of its structural properties. The frequencies of these modes were also determined.

h0008

Epitaxial strain effect on polarization and electronic structure of ferroelectric $Cu(OH)_2$

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We investigated the ferroelectric polymorphs of copper (II) hydroxide, starting from lattice instability of high symmetry (HS) Cmcm (SG.63). We noted that two different zone-center phonon branches corresponding to Branch-1 and Branch-3 (B_{1u} , I_2^-) lead to two different polar $Cmc2_1$ (SG.36) structures with different degrees of polarization. In this work, we investigate ferroelectric polarization and electronic structure of layered copper (II) hydroxide under epitaxial strain using first-principles calculations. Our calculations predict this as an indirect wide bandgap (WBG) semiconductor and variation of band gap as a function of epitaxial strain is also presented. The spontaneous polarization increases and decreases under compressive and tensile strain, respectively, due to structural distortion.

h0009

Dielectric Relaxation Study of O-Chloro-Aniline and Methoxy Propane-2-olBinary Mixtures at DifferentTemperatures using Time Domain Reflectometry

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The dielectric relaxation dynamics of O-Chloro-aniline in methoxy propane 2-ol is accurately measured at a wide range temperature for all concentrations and different volume fractions by pulse TDR using Tektronix DSA8300 Digital Serial Analyzer with the 200 KHz signal. The volume relationship of an entity is elucidated by the results in dielectric properties about the same. The static dielectric constant and excess relaxation time exhibit an increment whereas relaxation time and excess static dielectric constant observed decrement with increasing volume fraction. These findings suggest a complex interplay between the solute-solvent and the role of ether linkages in alcohol molecules. Finally, the Bruggman factor from the above mixture at different volume fractions which too approaches unity are reported to provide insight into the microstructure evolution of mixtures. These results bring about some new knowledge concerning the dielectric relaxation behavior of O-Chloroaniline and Methoxy Propane-2-ol binary mixtures which would be very useful for many technological applications.

h0010

Structural, Magnetic and Dielectric Study of $Bi_2Fe_4O_9/CoFe_2O_4$ Composite

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Composite $Bi_2Fe_4O_9$(90)/$CoFe_2O_4$(10) was synthesized using the sol-gel auto combustion method. The structural, magnetic, and dielectric characteristics were studied in the present work. The crystallite size of composite ~ 60 nm was calculated from the Rietveld Refinement analysis of room temperature X-ray diffraction (XRD) patterns. Surface morphology depicted the inhomogeneity in grain dispersion with 0.7µm-sized grains on average. The field-dependent magnetization curve at room temperature (RT) showed weak ferromagnetism with a saturation value of ~ 8 emu/g by applying an external field ±15 Oe. Temperature dependence dielectric study at constant frequencies showed the transition near 300 K, revealing the presence of MD coupling. MD coupling provides an extra degree of versatility in multifunctional device usage and creating innovative sensors, actuators, and memory devices.

h0011

Microwave Sintered Ternary BCST Ceramic with Sub-Zero Curie Temperature for Low Temperature Switching Application

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Cold-weather surface wind measurements have become an increasingly important source of information for weather forecasters and combat pilots. The purpose of this study is to investigate microwave-sintered ($Ba_{0.945}Ca_{0.055}Sn_xTi_{1-x}$) O_3 (BCST) ceramics with $x = 0.08$, with a particular emphasis on the structure, microstructure, and electrical properties of the material. By conducting Rietveld refinement investigations on the sample, it is determined that the perovskite structure and tetragonal phase are really present. Ceramics with $x = 0.08$ that have a high dielectric constant of 25,396 at 1 kHz and a low Curie transition temperature (T_c) are appropriate for use in applications that need low temperatures because of their combination of these two characteristics. Additionally, the ac conductivity as function of temperature is examined. A low-temperature conductivity zone as well as a high-temperature conductivity region were evident in the material that was examined. An Arrhenius plot is utilised in order to ascertain the activation energies of BCST ceramic substrates.

h0012

High-Temperature Electrical Properties of Lead-free 0.78NBT-0.2ST-0.02KNN Ceramic

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New age electronic market demands environment-friendly dielectric materials that can operate effectively at high temperatures. In this regard, we have attempted to investigate a morphotropic phase boundary (MPB) composition $0.78Na_{0.5}Bi_{0.5}TiO_3$ -$0.2SrTiO_3$-$0.02K_{0.5}Na_{0.5}NbO_3$ using Complex Impedance Spectroscopy (CIS) over a temperature (400- 650ºC) and frequency range (1 Hz to 1 MHz). Contribution of grains and grain boundaries towards electrical properties is adequately explained using complex impedance data. Studies on the frequency dependent real Z* and Im Z* provide important insight into relaxation and conduction mechanisms. Temperature dependent conductivity analysis was performed and corelated the conductivity study with impedance study to understand the electrical properties at high temperature.

h0013

Wind Energy Harvester Based on Electrospun CNT/DNA Doped Poly(vinylidene fluoride co hexafluoropropylene) Composite Nanofibers

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Composite nanofibers (NFs) of CNT and DNA doped electrospun poly(vinylidene fluoride-co-hexafluoropropylene) [P(VDF−HFP)] are prepared for designing the ultrasensitive wearable piezoelectric harvester (WPH). The fabricated piezoelectric harvester from the composite ES(CD-HFP) NFs mat demonstrates better output performance with an open circuit voltage output of ~12 V under a pressure amplitude of ~14 kPa and output power of 5.6 μW. A wind blower associated with the composite nanofibers (NFs), a wind velocity of ~8.5 m/s showing a maximum of ~4.5 V of open-circuit output voltage, and the ability of successfully charging up capacitors promising for developing wind energy harvesting applications.

h0014

Enabling Ferroelectric Polarization in CMOS Compatible Aluminium Nitride Thin Films with Scandium Alloying

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AlN is a non-ferroelectric piezoelectric material with a moderate piezo response compared to other piezoelectric materials. Nevertheless, doping or alloying suitable elements, such as Scandium, can overcome this drawback. The doping of Sc induces spontaneous polarization by reducing the barrier height for ferroelectric switching, along with the enhancement of the piezoelectric properties of AlN. In this work, we report on the deposition and ferroelectric characterization of AlScN thin films. The deposited AlScN thin films have intense (002) peaks with columnar growth. A distinct resistive switching mechanism was observed in the films grown at Sc sputtering power of 100 W. The introduction of Sc enhances ferroelectric polarization, which increases with Sc concentration. These findings further validate the highest polarization of 38.41 μC/cm2 seen for the films deposited with a Sc power of 100 W, making it a preferential candidate for ferroelectric applications.

h0015

Low Temperature Dielectric Relaxation and Impedance Spectroscopy Evaluation in $0.7(Bi_5Ti_3FeO_{15})/0.3(La_{0.67}Sr_{0.33}MnO_3)$ Composites

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The present work reports the study of dielectric relaxation and impedance spectroscopy $0.7(Bi_5Ti_3FeO_{15})/0.3(La_{0.67}Sr_{0.33}MnO_3)$ composite. A sol-gel process is adopted to synthesize the composite ceramics. The presence of dual phases without any additional impurity phases is established from the Rietveld refinement of the XRD profile. The temperature variation of dielectric and impedance data is presented in permittivity and Nyquist formalism to understand the relaxation dynamics. The frequency vs. dielectric data shows more dispersive behavior above 150 K compared to the low-temperature region, which signifies that the relaxation mechanism is significant toward room temperature. The Modified Debye analysis is employed to estimate the exact origin of the relaxation mechanism around 150 K. Arrhenius analysis reveals two different activation energies (2.2 meV and 119 meV) are present below and above 150 K. The thermally activated hopping of electrons between the Fe^{3+}/Fe^{2+} and Mn^{3+}/Mn^{4+} sites is the primary cause of the relaxation. The impedance spectroscopy is employed to analyze the relaxation mechanism, which reveals that the direct dependence of dielectric relaxation with the grain capacitance lies in the composite.

h0016

Effect of annealing rate and annealing temperature on structural properties of PZT thin film

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Lead zirconate titanate (PZT) thin films are of significant interest in various technological applications, such as MEMS sensors/actuators and non-volatile memories, due to their exceptional piezoelectric and ferroelectric properties. In this work, PZT [$Pb(Zr_{0.52}Ti_{0.48})O_3$] thin films are deposited on $Pt/Ti/SiO_2/Si$ substrates using the sol-gel method. The deposited films are annealed at different temperatures (600, 650 and 700 ℃) and heating rates (2 and 10 ℃/min) to attain the perovskite phase formation. The heat treatment, including the baking (150 ℃) and conventional annealing, develops thermal stresses at the interface due to the difference in the thermal expansion coefficients of PZT and the interlayer materials. We systematically investigated the effect of annealing temperature as well as the rate of annealing on the structural properties of PZT thin films, using x-ray diffraction and Raman spectroscopy.

h0017

Synergistic Enhancement of Energy Storage Properties in 2D-3D Composites of Graphene and Barium Titanate

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Two-dimensional (2D) material-based composites have gained a lot of attention due to their ability to increase polarization properties, which are crucial for advanced flexible electronic applications. In this study, we explore the synergistic effect of graphene (G) on the polarization properties of Barium titanate ($BaTiO_3$ (BT)). The G-BT nanocomposites were synthesized utilizing the microwave-assisted solid-state method. XRD analysis reveals distinctive peaks of graphene and BT in G-BT composites. The addition of graphene enhances mechanical stability and reduces the flow of unwanted charge carriers, therefore increasing the overall ferroelectric behavior of G-BT composites. As a result, we observed an increased recoverable energy storage density, Wrec, of approximately 135.97 mJ/cm³ and 167.06 mJ/cm³ for 5 wt% and 10 wt% of graphene in BT, respectively. Additionally, the breakdown voltage (Eb) increases significantly from 38.2 to 52.71 kV/cm. Overall, combining graphene with BT yields composites with better polarization properties, making them attractive for advanced electronic and flexible ferroelectric applications.

h0018

Temperature Induced Phase-Shift in Cobalt Substituted $KBiFe_2O_5$

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Recently emerged $KBiFe_2O_5$ compound exists in different space groups depending on the synthesis route. In this manuscript, the transition element cobalt (Co) is substituted at the iron (Fe) site of $KBiFe_2O_5$ (KBFO), and the 5% Co-substituted KBFO ($KBiFe_{1.95}Co_{0.05}O_5$: KBFCO) is investigated with temperature. The KBFCO sample is prepared following the conventional solid-state reaction route. The room-temperature X-ray diffraction study confirms the phase purity of the prepared sample having a monoclinic structure in the P2/c space group. Temperature-dependent dielectric and magnetic analysis (250 K to 510 K) is performed to identify the observed phase transitions. Temperature-dependent Raman study is performed from 120 K to 420 K to verify the observed phase transitions. However, the temperature-dependent dielectric, magnetic, and Raman properties of KBFCO reveal an anomaly near about 420 K. It shows a Raman shift of the particular modes related to Fe-tetrahedral near 420 K. It is expected that the observed anomaly near about 420 K, a phase shift for KBFCO compound.

h0019

Tuning The Structural And Dielectric Properties Of $Ba_{0.5}Sr_{0.5}Fe_{12}O_{19}$ Through Fe/Sr Molar Ratio

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The Ba doped strontium hexaferrite ($Ba_{0.5}Sr_{0.5}Fe_{12}O_{19}$) was prepared using the standard solid-state reaction method by varying the Fe/Sr molar ratios to 11 and 12. X-ray diffraction and dielectric measurements were carried out on the prepared samples to study their structural and dielectric properties. Rietveld refinement on the X-ray diffraction data reveals the formation of single phase magnetoplumbite structure of the prepared ferrite and it belongs to $P6_3/mmc$ space group. The reduction in crystallite size and enhancement in porosity was observed for the sample with an 11 molar ratio, which resulted in the enhancement of the dielectric loss properties. Low dielectric constant and high dielectric loss factor were observed for samples having 11 molar ratios. For this sample, the tangent loss enhanced in the higher frequency region hence the AC conductivity must increase in the higher frequency range.

h0021

Photodetection In 2D/1D Hybrid System Via Piezo-Phototronic Effect

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This work demonstrates the photoresponse attributes of a 2D/1D system by integrating the charge transfer mechanism and the piezo-phototronic effect. When exposed to UV light, the current in the $B_xC_yN_z$ decorated device is higher than in bare ZnO. Furthermore, an enhanced charge transfer is indicated by the higher photoresponsivity of the $B_xC_yN_z$ decorated system under strained condition. The next generation may benefit from affordable, self-powered photodetectors with the advancement of such hybrid systems.

h0022

Hafnium Substituted Barium Titanate: Structural, Ferroelectric and Dielectric Study

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In the present work we report the study of Hafnium substitution effects on polycrystalline Barium titanate $BaTiO_3$ (BTO). Structural changes with substitution are studied using x-Ray diffraction (XRD) and Raman spectroscopy measurements. Temperature dependent dielectric measurement shows frequency dispersion with increasing Hf concentration (≥40%) at Ti site of BTO. Analysis of Raman spectroscopy data indicate the systematic transformation of long-range ferroelectricity to relaxor behavior with Hf substitution.

h0023

Comprehensive Exploration of Structural, Optical, and Dielectric Properties in Hydrothermally Synthesized SnMnTe Nanocubes

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Recently, the quickly expanding field of power electronics has placed a significant demand on dielectric materials with a minimum loss, extensive energy storage capability, and satisfactory temperature stability. In this work, we have examined the optical, structural, and dielectric characteristics of SnMnTe matrix by adjusting the amount of Mn and Sn. The sample was synthesized by utilizing the single-step hydrothermal method. By using X-ray diffraction, the structural characteristic of the compound was examined. It was found that material crystallizes in a cubic form. The Raman analysis also confirmed the polycrystalline nature of the prepared sample containing two phases, MnTe and SnTe. The sample shows high reflectance percentage for higher wavelengths. Simultaneously, the sample exhibit low bandgap value about 0.54 eV. The prepared sample have agglomerated nano sphere shapes, which are confirmed by the morphological analysis through FESEM. Investigating the dielectric characteristics with respect to temperature and frequency allowed for a thorough analysis of several parameters, including the electric modulus, dielectric constant, AC conductivity, and impedance spectroscopy. Applications for electronic and energy storage devices may benefit from the SnMnTe matrix's aforementioned optical, electrical, and dielectric characteristics.

h0024

Impact of Ni doping on structural and ferroelectric character of $BaTiO_3$ ceramics

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In this work, we have used the sol-gel auto combustion technique to synthesis undoped and nickel doped $BaTiO_3$ ceramics with the compositional formula $BaTi_{1-x}Ni_xO_3$ (x=0 and 8%). The confirmation of phase purity was done using the X-ray diffraction technique. The undoped sample is in a tetragonal phase with P4mm space group, while the doped sample is in both a tetragonal and a hexagonal phase within the P4mm and P63/mmc space groups, according to Rietveld refinement analysis. It implies that nickel doping has a significant influence on the phase transition from tetragonal to hexagonal. The Rietveld refinement approach is used to estimate a variety of unit cell properties, including lattice parameters, cell volume, bond length (Ti-O), and bond angle (Ti-O-Ti). The fluctuation in these parameters is caused by the deformation that the lattice experiences due to Ni doping. Using Scherrer's equation, the average crystallite was determined to be between 37 and 51 nm in size. The pristine sample possesses maximal levels of polarization parameters (Pr, Pm and Ec) that fall down with Ni doped sample.

h0025

Comparative Simulation of Piezoelectric Output at Different Inclinations in ZnO, $BaTiO_3$, and PZT-4 Nanorods for the Development of Tactile Sensors

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This study investigates the potential of three piezoelectric materials Zinc Oxide (ZnO), Barium Titanate ($BaTiO_3$), and Lead Zirconate Titanate (PZT-4) by varying the inclination angle of a cylindrical nanorod. The peak value of the piezoelectric potential of ZnO and $BaTiO_3$ nanorods is observed at 60° inclination angles with value 62.336 mV and 29.024 mV, respectively whereas in PZT-4 it is observed at 30° inclination angle with value 21.341 mV. Among these materials, ZnO nanorods exhibit higher piezoelectric potential at all relative inclination angles. The vertical nanorods in all the materials show less piezoelectric output, which contrasts with the existing assumption where maximum piezoelectric potential response should be observed in vertical nanorods due to higher d_{33} piezoelectric coefficient along the vertical direction. The values of piezoelectric coefficients and dielectric constant vary due to the anisotropic nature of the material. The higher piezoelectric output in inclined nanorods of all the material suggests increased normal stress and shear stress contribution. These results can be used for the development of efficient, highly sensitive, and better-performing tactile sensors.

h0026

New Oxygen Deficient Double Perovskite Ceramic Compound: $YSrCuFeO_5$

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In the present communication we have reported the (structural, impedance and conductivity) behaviour of a new oxygen deficient double perovskite $YSrCuFeO_5$ of the general formulae $A_nB_nO_{3n-1.}$ It has been synthesized using cost-effective mixed-oxide solid-state reaction route. Room temperature X-ray diffraction studies reveals the overall phase and further analysis suggests tetragonal symmetry with lattice parameters a = 3.8318(4)Å, c = 7.6063(4)Å and volume = 111.68(Å)^3. Microstructure study using scanning electron micrograph (SEM) confirms the formation of compact and homogeneously distributed grains with distinct grain boundaries with an average grain size of 1.32 µm. The crystallite size of the sample is calculated from the W-H plot and is found to be 63.9 nm. Non-overlapping small polaron tunneling (NSPT) and correlated barrier hopping (CBH) conduction mechanisms are prevalent in the sample. Complex impedance spectroscopy study suggests negative temperature coefficient of resistance (NTCR) behaviour and the deviation of the center of the semicircular loops from the real abscissa suggests Non-Debye type relaxation.

h0028

Investigation Of Structural And Dielectric Studies Of Ho Substituted Nd_2CoMnO_6 Double Perovskite Compounds

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In this article, we present a detailed investigation of the $(Nd_{1-x}Ho_x)_2CoMnO_6$ (x = 0.0 – 0.3) (NHCMO) series. Our research thoroughly analyzes the structural properties, dielectric, impedance, and conductivity properties of the NHCMO series. The samples were synthesized using a solid-state reaction technique, and their single-phase nature was confirmed through X-ray diffraction (XRD) analysis. From Rietveld refinement, it was found that all samples were found to have a monoclinic structure with the $P2_1/n$ space group. Frequency-dependent impedance studies reveal significant contributions from space charge polarization, while temperature-dependent measurements show a negative temperature coefficient of resistance Analysis of the frequency-dependent conductivity data using Jonscher's Power Law suggests that large polaron tunneling model effectively describes the conduction mechanism in the NHCMO samples. The activation energy (Ea) is calculated for both the relaxation dynamics and conduction process using the Arrhenius relation.

h0029

Evidence of Magneto-electric Coupling in Y-type Hexaferrite $Ba_2Mg_2Fe_{12}O_{12}$

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In this work polycrystalline Y-type hexaferrite Ba2Mg2Fe12O22 (BMFO) was synthesized using the sol-gel auto-combustion method. Room temperature Rietveld refinement of the X-ray diffraction pattern confirms the phase purity

with hexagonal crystal structure (R-3m space group). Temperature dependence DC electrical resistivity suggested polaronic hopping conduction. The activation energy was calculated 0.21 eV which is the same for both the cases with field (1T) and in the absence of field. It was evident that BMFO shows zero magnetoresistance. Temperature dependent dielectric study attributes the ferroelectric transition at ~ 520 K. Temperature-dependent magnetic study observed the phase change at T_C ~ 515 K. Field dependent magnetization study observed the maximum saturation magnetization of 18.39 emu/g in the presence of ±1.5 T. Dielectric and magnetic data appearing nearly same temperature, which indicates the presence of magneto-electric (ME) coupling in the compound.

h0031

Correlation Of Charge Conduction Dynamics With Structural Distortion In Dy-doped $CaBaFe_4O_7$

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$CaBaFe_4O_7$ is a magnetoelectric material that crystallizes in the $Pbn2_1$ space group and exhibits a layered structure with alternately arranged kagomé and triangular layers of FeO_4 tetrahedra, characterized by strong distortion. The material exhibits robust ferrimagnetic moment along the *c*-direction below its T_C at 275 K, and strong electric polarization monotonously increasing with field along the *c*-direction. Besides, the material is pyroelectric. We investigated the structure and conduction dynamics of a series of Dy doped materials – $Ca_{1-x}Dy_xBaFe_4O_7$ ($x \leq 0.05$), below 300 K, using temperature dependent high energy x-ray powder diffraction, dielectric analysis and electric conduction studies. We found that the ac conduction obeys overlapping large polaron tunnelling conduction model while the electric modulus obeys Havriliak-Negami model. Most interestingly, the electric modulus studies indicate cooperative dynamics of the polaron conduction which is strongly dependent on the structural distortion, tuned by the Dy doping.

h0033

Fabrication and Characterization of Fe_3O_4 /P(VDF-TrFE) Nanocomposite Films

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The Fe_3O_4 nanoparticles were prepared by chemical co precipitation method and these are found to be ferromagnetic at room temperature. The pure P(VDF-TrFE) and Fe_3O_4/ P(VDF-TrFE) composite films (30μm thick) were prepared via solution casting method. The proper ferroelectric hysteresis loop is observed for P(VDF-TrFE). The ferroelectric properties of these composite films were deteriorated for increasing volume fraction of Fe_3O_4 NPs because the sample becomes conducting due to the incorporation of nanofillers. P-E hysteresis loop indicates that voltage bearing capacity of these polymer nanocomposites deteriorates with the addition of magnetic nanofillers. The dielectric and loss tangent increases with increasing volume fraction of Fe_3O_4 due to the contribution of Maxwell-Wagner polarization effect between the interface of polymer and nanofillers. The I-V characteristic shows piezoelectric butterfly loops with two minima corresponding to ferroelectric nature of these films. The leakage current value increases with the increment in volume percentage of MNPs because the sample becomes conducting.

h0034

Tailoring of Electrical Properties of [0.98KNLNS-0.02BNZSH] Lead-Free Ceramics through Variation in Sintering Temperature

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In this work, $0.98[((K_{0.4}Na_{0.6})_{0.94}Li_{0.06})(Nb_{0.96}Sb_{0.04})O_3]-0.02[(Bi_{0.5}Na_{0.5})(Zr_{0.8}Sn_{0.1}Hf_{0.1})O_3]$, [0.98KNLNS-0.02BNZSH] KNN based ceramic have been synthesized through the conventional solid-state sintering method. The effect of sintering temperature on the phase structure, bulk density and dielectric properties has been investigated systematically. The XRD analysis reveals a tetragonal phase for 1050˚C, while it is observed to be a coexistence of rhombhohedral–tetragonal (R–T) phase for sample sintered at 1075˚C, and orthorhombic-tetragonal (O-T) for 1100˚C.

The optimum electrical properties such as Curie temperature (T_c) ~400°C, maximum dielectric constant (ε_m) ~5090, dielectric loss (tanδ) ~0.3, piezoelectric parameter (d_{33})~120pC/N and the bulk density ~4.77g/cm^3 have been obtained for ceramic pallet sintered at 1075˚C and an enhanced thermal stability coefficient also observed for the sample sintered at 1075°C.

h0035

Broad Temperature Dependent Dielectric Study of Sm-substituted $YCrO_3$ Perovskite

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This work studies crystal structure and dielectric relaxation behaviour in $Y_{1-x}Sm_xCrO_3$ ($0 \leq x \leq 0.3$) compositions characterized through X-ray diffraction (XRD) technique and dielectric spectroscopy. XRD spectra reveal the phase purity of compounds, which are crystallized through distorted orthorhombic structures with the Pnma space group. With Sm contents, lattice cell volume increases due to cationic size mismatch, distorting the crystal structure. The temperature-dependent dielectric study is carried out at a broad temperature range of 80 K-525 K at different frequencies. Sm content shows that both the dielectric constant and tan loss increase, which may be attributed to increasing charge carriers at the interfaces, and reveals that these compounds show relaxor-type behaviour.

h0036

Structural, Magnetic and Dielectric Properties of $MnCr_{2-x}Fe_xO_4$ (x = 0, 0.30, 0.50)

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This paper reports the preparation of single phase samples of $MnCr_{2-x}Fe_xO_4$ (x = 0, 0.30, 0.50) and study of their structural, magnetic and dielectric properties. All the samples are found to crystallize in cubic spinel structure with $Fd\bar{3}m$ space group. The hysteresis loops recorded at 50 K indicate a shift from paramagnetic behavior in the x = 0 sample to ferrimagnetic behavior in the x = 0.30 and 0.50 samples, suggesting that Fe substitution strengthens superexchange interactions and increases the magnetic transition temperature. However, the magnitude of magnetization decreases as the Fe concentration increases. Complex impedance studies reveal a relaxation phenomenon, and the dielectric constant increases with higher Fe concentration.

h0038

Ultra-Low Frequency Detection and High-Pass Filtering in Titania-Enhanced Flexible Piezoelectric Nanogenerators for Human Motion Tracking

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The rising trend in fitness and overall wellness drives the development of IoT-compatible smart health gear with multifunctional sensors. This work explores the nucleating effect of TiO_2 nanoparticles on weight-modulated PVDF-HFP films (PT-5, PT-10, and PT-15) and prototype a sensing device with the film showing superior β-phase nucleation. The PT-10 film, with optimal polar β-phase, exhibits the highest remnant polarization (2Pr) and energy density of 0.36 μC/cm² and 22.3 mJ/cm³, respectively, at 60 kV/cm. The films act as high-pass filters above 10 KHz with low impedance and high AC conductivity. Impedance studies show effective interfacial polarization in the low-frequency region. The PT-10 sensor detects ultra-low frequency (25 Hz) from blood flow and muscle oxygenation, sensing voluntary joint movements and tracking motions like walking and running. The nanogenerator, activated by finger-tapping, powers LEDs and charges capacitors under 50 seconds. This sensor's real-time motion sensing and tracking capabilities are promising for smart wearables, sports biomechanics, and medical devices.

h0040

On Dielectric and Conduction Properties of Nb_6TeO_{17}

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In this abstract, Nb_6TeO_{17}, a complex oxide in Nb_2O_5-TeO_2 system, was prepared by solid state reaction and studied by impedance spectroscopy. Single phase sample could be obtained by appropriate temperature and time conditions which is characterized by powder XRD and impedance spectroscopy. At high, frequency, the relative permittivity of about 27 was observed in a wider range of temperature. Both the real and imaginary parts of dielectric permittivity show an increasing trend with increasing temperature and decreasing frequency as typical ionic conductors. The dc-conductivity data extracted from real part of the ac-conductivity follow Arrhenius relation, while a change in slope around 350 K was observed. Activation energy for conduction is decreases from 0.73 eV to 0.55 eV around this temperature.

h0041

Ce and Bi Doped BCZT Based Lead-Free Ceramic: A Material with High Dielectric Constant

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In this study, perovskite type ($Ba_{0.95}Bi_{0.02}$ $Ca_{0.02}$) ($Zr_{0.02}$ $Ce_{0.0005}$ $Ti_{0.9795}$) O_3 (BBCZCeT) lead-free ceramic has been synthesized by conventional solid-state reaction method. X-Ray Diffraction (XRD) technique has been used to analyze the structural properties of the ceramic. The XRD analysis confirms that the synthesized material has a pure perovskite structure and no other phase or impurity is present. The dielectric study of ceramic shows that incorporation of Ce and Bi in BCZT results in a high dielectric constant of ~33182 and low dielectric loss of 0.17056 at 100 Hz at a reduced sintering temperature of 1360°C. Also, the phase transition peak is broadened and near relaxor behavior is observed.

h0042

Influence of Ag and Mg ions Substitution on the Structural and Dielectric Properties of Lead-Free $NaNbO_3$ Ceramics

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This paper reports on Ag and Mg modification's effect on the parent $NaNbO_3$ system. Lead-free and single-phase $Na_{0.85}Ag_{0.15}Nb_{0.95}Mg_{0.05}O_3$ solid solution is formed using most conventional solid-state reaction route. A comparative detail study on structural, microstructural, and dielectric properties of pure $NaNbO_3$ (denoted as pure NN) and $Na_{0.85}Ag_{0.15}Nb_{0.95}Mg_{0.05}O_3$ (denoted as Ag-Mg@NN(O_2)) is done in this report. The grain size of Ag-Mg@NN(O_2) is reduced to 2.853 µm and density is improved whereas pure NN has a grain size of around 5.503 µm with low density. The dielectric behavior of Ag-Mg@NN(O_2) is explained over a range of temperature (Room Temperature to 500 ºC) and frequency (1 KHz to 1 MHz). The presence of phase transition of Ag-Mg@NN(O_2) with varying temperature and frequency is studied from the temperature-dependent dielectric curves. The role of substituted Ag and Mg ions in the parent NN system is explained from XRD, SEM, and dielectric curves.

h0044

$La_{1.80}Y_{0.20}CuMnO_6$ Double Perovskite System: A Comparative Study of Techniques for Measuring Crystallite Size

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The double-perovskite compound $La_{1.80}Y_{0.20}CuMnO_6$ have been synthesized using a solid-state reaction method to understand the response of its structural properties. The structural parameters obtained by Rietveld refinement confirms that the sample crystallizes in orthorhombic structure in *Pnma* space group X-ray diffraction confirms its orthorhombic structure in the P*nma* space group. Analysis of crystallite size and strain was done using various methods like Debye-Scherrer, modified Scherrer, Williamson-Hall and Size- Strain method revealing an average size. Yttrium doping caused lattice distortion impacting symmetry and band configuration confirmed by the increased lattice parameters.

h0045

Synthesis and Characterization of Eco-friendly $NiFe_2O_4$ Octahedrons Spinel Ferrite for Multi-Faceted Applications

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In this work, we explore structural, morphological, raman and optical properties of Green Synthesized Nickel Spinel Ferrite $NiFe_2O_4$ (NFO) using Azadirachta indica (Neem tree) leaves extract. The heat treatment method was utilized for green synthesis and the sample was calcined at 1100°C for 4 hours. The XRD confirms the formation of cubic spinel phase of polycrystalline NFO. The morphology was examined using SEM, which shows the formation of octahedrons, with the average particle size distribution at around 500 nm. FT-IR was used to confirms the presence of iron oxide and metal oxide bonds at the octahedral and tetrahedral sites. UV-Vis spectroscopy is utilized for optical properties which shows that it has a strong absorbance peak in visible region. From Kubelka-Munk function the band gap is measured at 2 eV. Raman spectra confirm 5 raman active modes.

h0048

Fabrication and Characterization of Barium Hexaferrite Film Based Device for Neuromorphic Applications

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Hexaferrites, due to their unique magnetic and electrical properties, show great promise in multifunctional devices. This paper aims to study the electrical properties of Gold//Barium Hexaferrite//Graphite devices deposited on Alumina substrate—furthermore, structural analysis of the $BaFe_{12}O_{19}$ film by XRD and Raman spectroscopy at room temperature. The electrical characteristics are measured using Keithley SMU 2604B.The memristor device Alumina//Gold//Barium Hexaferrite//Graphite show bipolar analog switching behavior with an on/off ratio of 4.3.

h0049

Near Room Temperature Dielectric Relaxation in Lead Free $0.67BiFeO_3$-$0.33BaTiO_3$ (BF-33BT) Piezoceramic

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Among lead free perovskite piezoelectric, $BiFeO_3$ based piezoceramics have garnered enormous attention for exhibiting high T_C as well as room temperature antiferromagnetism. Particularly, $BiFeO_3$-$BaTiO_3$ solid solutions have become potential candidates as these exhibit morphotropic phase boundary (MPB) and high T_C value. Here, we report dielectric spectroscopy of BF-33BT ($0.67BiFeO_3$-$0.33BaTiO_3$), a MPB composition in a broad temperature (100-520 K) and frequency (10 Hz to 1 MHz) range, which shows ferroelectric relaxation around room temperature, manifested from dispersion in relative dielectric permittivity and a broad peak in loss tangent (tanδ). Origin of the ferroelectric relaxation has been identified as temperature dependent contributions of grain boundaries in polarization at low frequencies, which is dominant at higher temperatures and freezes slightly below room temperature.

h0050

Effect of Calcium and Zirconium Doping in Lead-free $BaTiO_3$ Ceramics for Energy Storage Properties

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Dielectric capacitors are playing an important role in the modern technology due to its high-power density and fast discharge rates. This article presents the study on, effect of Ca^{2+} and Zr^{4+} doping in A and B sites of lead free ceramics

$BaTiO_3$ (BTO) to form a $(Ba_{0.625}Ca_{0.375}Zr_{0.015}Ti_{0.985})O_3$ (BCZT) ceramics via solid state reaction method. XRD results confirms the formation of the tetragonal phase in both ceramics samples around room temperature. The ferroelectric to paraelectric phase change occurs at T_C =137ºC, that is confirmed by the sharp peak from the dielectric *Vs* temperature spectrum and the dielectric constant decreased with doping Ca^{2+} into the BTO lattice. Further the prepared BCZT ceramics investigated for the ferroelectric and energy storage properties and resulted in the maximum recoverable energy density of U_{rec} = 67.6 mJ/cm^3 with an enhanced efficiency of 66.6 % at 40 kV/cm.

h0051

Multiferroicity and Magneto-capacitance in $BaTi_{1-x}Fe_xO_{3-\delta}$ (x= 0, 0.02, 0.1, 0.15 and 0.2)

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In this report, we tried to find out the way to increase the magnetoelectric coupling in single phase $BaTi_{1-x}Fe_xO_{3-\delta}$ system. For this, all the magnetic orderings in the system were separately scrutinized through Mössbauer spectroscopic studies revealing the hyperfine parameters for the magnetic orderings perhaps for the first time for this system. Through the work, we proposed that oxygen vacancies play the key role in inducing magnetic orderings among the magnetic ions in the system. Presence of oxygen vacancies in three charge states were found in all the samples and the density of oxygen vacancies increased with increase in doping. The room temperature Mössbauer spectroscopy corroborates with the magnetic field dependence magnetization curves for every sample regarding the occurrence ferromagnetic and antiferromagnetic orderings along with the paramagnetic moment of the Fe^{3+} ions which are situated at the Ti sites in octahedral and pentahedral sites. Magneto-capacitance measurements revealed that the relative change in capacitance with magnetic field (MC) in Fe doped samples enhanced with increase in doping amount, about 41% for 10% doping. The MC that we obtained in the present work is found to be much higher than the earlier works of this $BaTi_{1-x}Fe_xO_{3-\delta}$ system.

h0052

Variation in Dielectric Properties of Sm^{+2} Doped Lead Titanate Prepared by High Energy Ball Milling

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Our aim and expectation is that modification of rare earth element as Sm^{+2} will be more dependent on the radii difference. Sumarium has selected as source of the guest ion. Such type of the studies has been reported hardly as such lead titanate having perovskite structure has been selected as host lattice. Powder form of the ceramic has been fabricated by using High Energy ball Milling (HEBM) method. Undoped lead titanate has minimum dielectric constant and increases gradually (with increasing rate of doping) by 5% of Sm^{+2} doped sample. From the figure it also appears that Tc shift to higher temperature side for 5% Sm^{+2} sample of doping concentration. Electrical conductivity measurements are reported. Doping with Sm^{+2} result in a marked reduction in particle size and unit cell volume of pure lead titanate. Partial substitution of the Sm^{+2} on the B- site suggested.

h0055

Mechanism of pressure tuning of ferroelectricity glycine silver nitrate – probed using infrared spectroscopy

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Glycine silver nitrate (GSN) is the first silver or nitrate ion based organometallic compound that showed ferroelectricity, with Curie temperature (T_c) of -55ºC. Based on various structural studies, it is believed that the ferroelectric transition in GSN is caused by the low-temperature mobility of silver atoms in the crystal. The only high pressure study, using dielectric measurements, have shown decrease in T_c with pressure. Here, using *in-situ* high pressure infrared spectroscopic investigations, we have shown the weakening of interatomic interactions between Ag and O atoms of nitrate as well as glycine-carboxylate groups with pressure. Consequently, a larger contraction of structure is required due to the elongation in the silver ion coordination lengths. This provides the mechanism of pressure tuning of ferroelectricity in GSN.

i) TRANSPORT PROPERTIES AND SEMICONDUCTOR PHYSICS

i0001

Defects correlated transport properties of modified $BaTiO_3$

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Crystal structure, bandgap, and the changes in the charge conduction mechanisms in ceramics are interrelated, and the underlying physics unifies all these different phenomena. The experimental evaluation of the electronic properties and ac conduction mechanism of $BaTiO_3$ and $Ba_{0.938}La_{0.062}Ti_{0.9375}Fe_{0.0625}O_3$ is attempted in this work. Bandgap was observed to be tunable with La/Fe doping from 3.2eV (x=0) to 2.6eV (x=0.062), while the lattice disorder was found to increase. Such changes in the electronic properties were confirmed from AC- conductivity studies. From different transportation models, Carrier Band Hopping is a preferred mechanism in the less distorted $BaTiO_3$. However, a Large Polaron Tunneling process can be justified for the doped samples. A transition from short range to long range conduction of charge carriers has been obtained from imaginary part of impedance and modulus spectra.

i0002

Investigation Of Charge Transport Properties Of RGO-CuSe-Based Schottky Diode By Tuning Graphene Content

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Here, we have reported the charge transport properties of reduced graphene oxide-copper selenide (rGO-CuSe) based Schottky diodes by tuning the rGO content over bare CuSe. The diodes showed better performance after incorporation of different weight percentage of rGO, among which the best result was obtained for 5% rGO content. Space charge limited current theory was used to determine charge transport properties like carrier mobility, transit time, and diffusion length. For 5% rGO incorporation, we have achieved a carrier mobility of 8.60×10^{-5} $m^2V^{-1}s^{-1}$ with a 38-fold increase over pure CuSe. The transit time was improved by 22 times and the diffusion length also increased by 30%.

i0006

Electron-Phonon Interaction Effects on Electronic Transport in "Bite" Defective Graphene Nanoribbons

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In this study, we have numerically calculated the electronic transport through "Bite" defective armchair graphene nanoribbons (AGNRs) when electron-phonon interaction is considered. In the case of "Bite" defective 8-AGNR, we observe a decrease in transmission with an increase in electron-phonon interaction strength but it does not become zero. The overall transmission decreases in the case of "Bite" defective 9-AGNR with an increase in electron-phonon interaction strength, but transmission shifts towards the centre of the band gap and remains zero near zero-energy.

i0007

Dependance on alkyl chain-length on the dynamics of (alkylamides+$LiClO_4$) Deep Eutectic Solvents

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In this study, we investigate the dynamics of $RCONH_2$ + $LiClO_4$ based deep eutectic solvents to elucidate the influence of chain length on molecular diffusion. The solvents examined include acetamide, propanamide and butyramide. Molecular dynamics within these DES were probed using quasielastic neutron scattering (QENS) and classical molecular dynamics (MD) simulations. Our study demonstrates that the dynamics in DESs consist of two components arising from jump diffusion of the COM and localised diffusion within transient cages. Analysis reveals that alkyl chain length critically impacts diffusion behavior within DESs. Specifically, an increase in chain length corresponds to a decrease in the jump diffusion component, while localized motions significantly contribute to the overall dynamics. Additionally, the size of the transient cages expands with longer alkyl chains.

i0011

Novel TCAD Approach Precisely Simulating Charge Collection Efficiency of 4H-SiC Alpha-particle Detectors

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This work reports a precise physics-based TCAD model for simulating charge collection efficiency (CCE) of 4H-silicon carbide (4H-SiC) Schottky barrier diode (SBD) alpha-particle detectors. The simulation results agree well with the state-of-the-art I-V and CCE characteristics of Ni/4H-SiC SBD detectors. Initially, the forward I-V is matched by fine-tuning physical parameters; then the reverse I-V characteristics are validated by employing a trap-assisted tunneling (TAT) model at the deep-level trap at EC – 0.73 eV. To make the simulation more realistic, the 5.486 MeV 241Am alpha-particle-induced electronic energy loss in SiC is computed by SRIM simulation. Subsequently, the linear energy transfer (LET) data calculated from SRIM is incorporated into the TCAD Heavy-Ion (HI) model. The conventional HI model can predict only the drift-induced charge portions of CCE, which is valid at higher detector bias voltages. Hence, a novel approach is adopted to include both drift- and diffusion-induced transient currents in the detector response; thereby the CCE of the detector is accurately simulated over a wide voltage range (0 V to -250 V).

i0012

Thermal Annealing Induced Enhancement of Electrical Performance in PDMS Assisted Exfoliated multilayer MoS_2 based Field Effect Transistor

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This paper investigates the effect of thermal annealing on the electrical properties of exfoliated multilayer MoS_2 based FET. To probe this effect of thermal annealing, the device was annealed at 200 °C for 2 hrs. We observed that off current decreased drastically by three orders of magnitude, increasing the $I_{on/off}$ ratio by three orders. Additionally, mobility increased by 2.5 times, the subthreshold swing reduced by a factor of 8, and hysteresis improved from 13 to 3.7 V. Molybdenum disulphide (MoS_2) was exfoliated onto SiO_2/Si substrate using polydimethylsiloxane (PDMS) stamp. The resulting Exfoliated MoS_2 flake was analysed using an optical microscope and Raman spectroscopy. For measuring electrical response, Output (I_d~V_d) and transfer (I_d~V_g) characteristics has been measured.

i0013

Highly Responsive HTL Free Self-powered Photodetector based on Ag/Bi co-doped $CsPbBr_3$ Nanocrystals

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Abstract. Doping and co-doping in metal halide perovskite have garnered significant attention because of their ability to tune the optoelectronic properties of the host materials. Herein, we have strategically utilized Ag and Bi as co-dopants in $CsPbBr_3$ nanocrystals to improve the optoelectronic properties of the host materials. Fabricated low-cost hole transport layer-free (HTL-free) photodetector (PD) with Ag/Bi co-doped $CsPbBr_3$ exhibited substantial photoresponse with a dark current to photocurrent ratio of 4.15×10^6, indicating efficient e-h pair generation inside semiconductors and subsequent dissociation in the respective electrodes. Furthermore, there is a remarkable enhancement of photocurrent, responsivity, and detectivity of about 900%, 600%, and 650%, respectively, compared to the pristine $CsPbBr_3$ photodetector. This innovative technique highlights the enormous potential of heterovalent codoping in lead halide perovskite to tune the optoelectronic properties, paving the way for efficient and cost-effective solutions for next-generation optoelectronic devices.

i0014

Synthesis and characterization of Bi-Doped CdTe Nanoparticles via hydrothermal synthesis for Optical and Photo-Response applications

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Due to various structural and optical properties, metal telluride nanomaterials are favorable candidates for different optoelectronic applications. This study describes a simple hydrothermal synthesis for Bi-doped CdTe nanoparticles, wherein four distinct samples are generated by adjusting the concentration of Bi doping. Structural analysis by X-ray diffraction (XRD) confirmed the presence of CdTe cubic phase in the material, with observable phase shifts due to Bi incorporation. Raman spectroscopy provided insights into different vibrational modes of CdTe, while transmission electron microscopy (TEM) analysis further elucidated CdTe phase and determined interplanar spacing values. The field emission scanning electron microscopy (FESEM) revealed a consistent nanoparticle-like morphology, unaffected even by increased Bi concentration. UV-Vis study revealed a decrease in the bandgap, indicating potential shifts in the material's optical properties. The photo-response study demonstrated an increase in current value, and alterations in rise and decay times of the material.

i0015

Thermoelectric Performance of Cubic Perovskite ($HfMgO_3$): A DFT Approach

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In this work, the density functional theory and semi-classical transport theory is employed to calculate the structural, electronic and thermoelectric properties of cubic perovskite oxide $HfMgO_3$ using PBE-GGA and TB-mBJ exchange-correlation functional. The band structure of this compound reports the indirect band-gap of 2.142 eV with a p-type semiconductor nature of the material. The transport properties i.e., the Seebeck coefficient, electrical conductivity, electronic thermal conductivity are calculated using constant relaxation time. Substantially, the Seebeck coefficient (232 μV/K) and low lattice thermal conductivity (8.64 W/m K) at 300 K are computed. The maximum Figure of Merit (ZT) is 0.35 at 1200 K which ensures the studied material is suitable in view of thermoelectric performance.

i0016

Co-existence of Ferro-Antiferromagnetism and Transport Properties in Full Heusler Alloy Fe_2MnAl

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Heusler alloys find their applications as sensors, actuators, energy harvesters, and as magnetic cooling devices. For the current study, polycrystalline ingots of fe2mnal samples were prepared by conventional arc melting stoichiometric amounts of constituent elements in a high-purity argon atmosphere and annealed at 800℃. These alloys exhibited a distinct magnetic transformation around 50k, attributed to antiferromagnetic pinning within a ferromagnetic matrix. The mixed state incorporates ferromagnetic and antiferromagnetic parts for which close-lying curie (tc) and néel (tn) temperatures can be identified from magnetization measurements. Noteworthy results included a semiconducting property below ~120 k (tc) and metallic behaviour above, as evidenced by temperature-dependent resistivity. Remarkably, a negative magnetoresistance arising from inhomogeneous magnetic scattering was observed within the same temperature range.

i0017

Electrical Transport Properties of $LaAl_2$ Single Crystal

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We report the crystal growth, structural characterization, and electrical transport properties of single crystalline $LaAl_2$. The compound is grown using Czochralski method. It crystallizes in cubic crystal structure (space group: *Fd-3m*, #227) with lattice parameter 8.147(6) Å. The compound is diamagnetic in nature. The metallic nature of the compound is verified from the electrical transport properties. The large residual-resistance ratio (RRR = 25) confirms the good quality of the crystal. We observe an intriguing behaviour of resistivity in $LaAl_2$ that remains independent of magnetic fields up to 14 T. The observation of quantum oscillation in the de Haas van-Alphen measurement ascertains the good quality of the grown crystal.

i0018

Cerium Doped $Cs_2AgInCl_6$ Microcrystals Towards Enhanced Self-Trapped Exciton (STE) Emission and Enhanced Optoelectronic Properties

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Doping in $Cs_2AgInCl_6$, a direct bandgap, broadband emitting, and highly stable semiconductor, has garnered widespread attention because of its highly tunable optoelectronic properties. This report encapsulates the key findings from various structural and optical measurements. Herein, we have synthesized cerium (Ce) doped $Cs_2AgInCl_6$ using halide precursor-based acid precipitation method. Our results unveil the exceptionally high emission intensity of 5% Ce doped $Cs_2AgInCl_6$. This high emission intensity is due to the Ce^{3+} ion which act as a potent luminescent core. Further, this material can be used for the as efficient future white light source.

i0020

Visible Light Response Photocatalytic Activity Appreciably Enhanced by Dy-Substituted $KBiFe_2O_5$

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Dye effluents released from various factories and industries causes environmental contamination as well as health hazards, so it is highly necessary to take care of this issues. This work sheds light on the worthwhile photodegradation of methylene blue (MB), a common industrial dye in Dy substituted KBiFe2O5 ($KBi_{1-x}Dy_xFe_2O_5$ (x = 0, 0.05, 0.075, 0.1)). KBiFe2O5 is a brownmillerite structured promising multiferroic photoactive material favorable for Photocatalytic and photovoltaic application. Solid state reaction method is adopted to synthesize Dy doped KBiFe2O5 and XRD analysis confirms the monoclinic structure with P2/c space group of the materials. Through rigorous optimization, the photocatalytic performance of doped sample is enhanced from 62% to 95% MB degradation efficiency under direct sunlight in 180 minutes. This study also explains the stability of the photocatalyst after two cycles photodegradation process. The photodegradation of dye is also achieved around 90% efficiency of 10%-Dy doped KBiFe2O5 upon testing in river water for practical application. Magnetic moment increases 5 times with Dy substitution.

i0023

Large Thermoelectric Power Factor in $Ni_2MnSn_{0.75}Al_{0.25}$

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We have examined the structural, transport and thermoelectric properties of $Ni_2MnSn_{0.75}Al_{0.25}$. X-ray diffraction measurement shows that the system crystallized in double phase with Fm-3m and Pm-3m space group. The temperature-dependent electrical resistivity behavior indicates that $Ni_2MnSn_{0.75}Al_{0.25}$ is metallic in nature. The Seebeck coefficient suggested that n-type behavior over the whole temperature range with a large power factor.

i0024

Field Tunable Temperature Sensitivity of a Pulsed Laser Deposition Grown Manganite-Based Sensor Device

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Temperature sensitivity is essential for designing, operating and maintaining various electronic systems to ensure their function reliably within specified parameters and requirements. Manganite based materials are very popular due to their properties such as Colossal Magnetoresistance (CMR), Electroresistance, Metal-Insulator transition, high sensitivity, stability and reliability which make them stand out for wide range of applications such as thermoelectric

devices, magnetic sensors, memory devices, spintronics, etc. In this communication, we report the sensing capabilities of manganite-based $Y_{0.95}Ca_{0.05}MnO_3$ (YCMO)/Nb:$SrTiO_3$ (SNTO) (*100*) device fabricated using sophisticated Pulsed Laser Deposition (PLD) technique. Structural properties were studied by X-Ray diffractometer based (θ-2θ and Φ-Scan) measurements and microstructural properties were studied using AFM. The temperature sensitivity of the device was studied by Temperature Coefficient of Resistance (TCR) with varying temperature from 100K to 300K and voltage up to 2.0V by using the Keithley make 2612 A source meter attached with a cryostat. It showed the semiconducting nature from the negative value of TCR along with enhanced sensing capabilities at lower temperature which makes them better for low temperature sensing applications. Also, it was observed that its sensing is enhanced by application of external electric field. Therefore, these investigations strongly support the capabilities of manganites-based devices for temperature sensing applications.

i0025

Structural and Electrical Insights into Bulk and Nano $La_{0.67}Ba_{0.33}MnO_6$ Manganite

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This paper compares the structural and electrical-transport characteristics of bulk and nano-$La_{0.67}Ba_{0.33}MnO_3$ manganite. Rietveld refinement confirms rhombohedral phase crystallization in both samples within the R-3c space group. At low temperature region below 50 K, resistivity data indicates Kondo-like transport behaviour. The metal-insulator transition (T_{MI}) in the nano sample shifts to approximately 200 K due to increased electron-electron scattering at grain boundaries with decreasing grain size. In the ferromagnetic-metallic region, resistivity is influenced by grain/domain boundaries, electron-electron, and electron-phonon scattering processes.

i00026

Energy Efficient CdO/$La_{0.3}Ca_{0.7}MnO_3$/Al_2O_3 Volatile Memristive Device with Neuromorphic Resemblance

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Manganite based memristive devices have shown a great response towards their operations as a volatile and non-volatile resistive switching characteristics, which are the essential requirements in the newly emerged field of neuromorphic devices. CdO/$La_{0.3}Ca_{0.7}MnO_3$/Al_2O_3 heterostructures have been prepared using cost effective spin coating technique. CdO and $La_{0.3}Ca_{0.7}MnO_3$ (LCMO) both are known to be n-type semiconductors, make the n-n junction based heterostructure, where this bilayered geometry was grown on the Al_2O_3 substrate. The electron doped LCMO exhibits charge-ordered phase, exhibiting a sharp rise in resistivity below the transition temperature. Temperature dependent resistive switching measurements have been performed which shows the temperature induced shifting in threshold and holding voltages. All the measurements showcase volatile nature of resistive memory and, thus, can function as resistive random-access memory (ReRAM). This volatile memory (VM) storage nature also resembles to certain elemental functionalities of neurons and, hence, these heterostructures can act as a neuromorphic system when systematically connected in a cascaded matrix of memory cells. This memristive device consumes very low power by taking advantage of selector configuration based on its resistive states, which can completely stop sneak-path leakage current that was a major issue in the traditional crossbar architecture of memory cells, otherwise.

i00027

Synthesis and Magneto-transport Properties of Pd_3In_7: A Topological Dirac Semimetal

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Dirac semimetals have gained attention due to their unique electronic properties and potential applications in advanced electronic devices. Here we report the synthesis and characterization of the polycrystalline Pd_3In_7 and study the transport properties of the sample. Pd_3In_7 has a body-centric cubic lattice structure with space group $Im\bar{3}m$ (Space group no 229). The temperature-dependent resistivity measurements reveal a linear behaviour at high temperatures

(T>50K), indicative of dominant electron-phonon scattering at that temperature range. For T<50K, it follows quadradic dependence on temperature T, suggesting the Fermi liquid behaviour. The linear magnetoresistance (MR) of 402% at 20K and 5T, suggests the presence of Dirac fermions in the polycrystalline Pd_3In_7.

i0028

Surface Morphology of Sb Based III-V Semiconducting Substrates Grown by VDS

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Antimony based III-V semiconducting substrates were grown by Vertical Directional Solidification mechanism. Since electrical properties are sensitive to defects, substrates' to-be-doped surfaces were characterized prior to their application as device. AFM, XRF, SEM, EDAX and EDAX elemental mapping tools were used for determination of roughness, stoichiometry and absence of oxidation. Comparison of the surfaces exhibited by different binary and ternary VDS substrates and their morphological ability to be doped is reported here. For GaSb (34.5,65.4) and InSbBi (48.1,48.7 and 3.21) mass % agrees the stoichiometry. Some defects are Bi rich (~30%) pockets of 1μm exhibiting non-assimilation of Bismuth in InSb lattice and clustering locally. Surface roughness (rms) determined by AFM is 12.25 and 12.65 Å for GaSb and InSbBi respectively. Numerous 1 mm^2 implantable regions are available for doping. In all cases uniformity in area constitutes more than 2/3rd fraction of polished surface.

i0029

Bioelectronic Non-volatile Memristive Device with Supreme Endurance

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Due to the overuse of dangerous materials, electronic waste has become an unwanted burden on our environment as a result of technological advancements. Utilizing biomaterials to create electronic devices that are non-toxic, ecologically friendly, and biocompatible is therefore very advantageous.Resistive Random Access Memory(RRAM) is one of the most promising memeristive device due to its simple metal-Insulator-Metal(MIM) structure, having high-speed, ultimate scalability, low power consumption, capability of numerous-bit switching and CMOS compatibility. Here, we have highlighted the conduction mechanism in a *Polysaccharide gel-based* MIM structured bioelectronic memory device.2-probe I-V transport measurements have been done to investigate the switching ability. The coexistence of NDR with bipolar resistive switching is observed. SCLC conduction mechanism dominates the conduction mechanism of the system device demonstrates supreme endurance over 500 consecutive switching cycles with a maximum ON/OFF ratio of 10^3.

i0030

Vertical Schottky Barrier Diodes fabricated from $ZnGa_2O_4$ epilayer grown by MOCVD

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Abstract: In this study, we have fabricated vertical Schottky barrier diodes (SBD) based on $ZnGa_2O_4$ epilayer grown by MOCVD on the highly doped bulk $ZnGa_2O_4$ substrate. The electrical properties of the SBD were investigated. The SBD showed an ideality factor of about 1.51 with a forward On voltage of 0.275 V. Additionally, the On/Off ratio was found to be 10^4 with a breakdown voltage of 8.5 V. The highly doped bulk substrate SBD performance was improved by depositing $ZnGa_2O_4$ epilayer. The results present the use of $ZnGa_2O_4$ for the power applications.

i0031

Intense Near Infrared Emission from Li Doped ZnO Crystallites

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Li doped ZnO crystallites have been synthesized by solid state reaction of ZnO powder and Li_2CO_3 at 750°C. Li has been successively doped up to 20 atomic percent without phase segregation. Lattice parameters of doped ZnO increase for Li concentrations up to 5 at.% and found to contract significantly for further increase in doping level due to the attractive field created interstitial lithium. An intense near infrared (NIR) emission from the Li doped ZnO is observed which was absent in pure ZnO. The NIR emission at low temperatures (below 10K) comprises of sharp lines indicating the presence of deep level Li related defects. When excited near the band edge, decay curves of these lines exhibit multiple components and can be characterized by an average lifetime around 5 ms.

i0032

Reason for Resistivity Upturn and Carrier Compensation in the $ZrAs_2$ Single Crystal

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Single crystals of $ZrAs_2$, which crystallize in the orthorhombic structure with nonsymmorphic space group, have been successfully grown by the flux method. The temperature dependent resistivity shows a metallic behaviour in the absence of a magnetic field, but a resistivity upturn is observed under a high magnetic field. Magnetoresistance does not saturate up to the 14 T magnetic field and reaching a relatively large value (1010% for $I \parallel [010]$, $B \parallel [105]$). The presence of two types of carriers in $ZrAs_2$ is indicated by the nonlinear Hall resistivity. The carrier concentration is derived from the field dependent Hall resistivity utilizing conventional two band model, and it is found that the charge carriers are nearly balanced, a key factor contributing to the observed large magnetoresistance. Furthermore, we have demonstrated a specific criterion for metals to exhibit a resistivity upturn in the presence of a magnetic field. Our first-principles calculations disclose carrier compensation on the Fermi surface, which plays a significant role in the large magnetoresistance observed.

i0033

Study of Variation in Properties of Bulk Crystals of Indium Antimonide Nitride with Time

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The required energy gap of infra-red detectors varies depending on their applications. Indium antimonide band gap at room temperature is 0.17 eV. An attempt was made to reduce the energy gap further by addition of nitrogen during the crystal growth. It was reported that the band gap reduces drastically, for 1 percent incorporation of nitrogen, the band gap reduces by 100meV while the lattice parameters remain unchanged. Three bulk crystals of dilute nitride of Indium antimonide were grown using vertical directional solidification techniques with atomic percentage of nitrogen as 0.1%, 0.2% and 0.5% respectively. These crystals were characterized again recently and the EDS study indicated reduction in percent of nitrogen. The XRD analysis does not show variation in the diffraction peaks. The compositional analysis results show one third of nitrogen in the compound has disappeared over the years. The study was further enhanced by Raman spectrum of the dilute nitride of Indium antimonide for changes in crystal quality and composition.

i0035

Microstructural, and Electrical Conductivity Study of Mg Doped Cobalt Ferrite for Thermistor Application

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This experimental study investigates the structural, electrical conductivity, and Thermistor properties of Mg-doped cobalt ferrite synthesized via the solid-state reaction method. The microstructural properties of the sample were studied, and the average grain size was calculated using Image J Software. The variation of conductivity with sample frequency satisfies Johnschrer's Power Law and confirms the negative temperature coefficient of the resistance behaviour of the material. All the values of thermistor properties, including thermistor constant, sensitivity index and activation energy, indicate the suitability of the sample for thermistor applications.

i0036

Electrical and Thermal Transport Properties of Eco-Friendly HB Graphite Conductive Paint along with its Applications for Printing Electronics

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A range of flexible electronics devices have been printed using different functional inks, such as metal nanoparticle inks, semi-conductive inks, and polymer inks. Our focus was on the development of carbon-based inks, since they offer significant benefits in terms of solution process ability, abundant nature, and low cost of production. In this work, we prepared HB graphite-based conductive paint using a novel approach and evaluated its electrical, thermal and sensing properties on flexible Xerox paper. Further, the electrical resistivity and thermopower was determined to be 0.0064 Ω cm and 12.34 μVK^{-1}, respectively, resulted in room temperature power factor of 540 $nW\text{-}m^{-1}K^{-2}$. This is the lowest order magnitude in resistivity of graphite conductive paint due to which it can be used for connecting the circuital breaks. We also found that it can function as both *p*-type and *n*-type after treatment with polymers like PEI and PVA (polyvinyl alcohol). After this treatment, the Seebeck coefficient is changed to -3.11 μVK^{-1} and -35.75 μVK^{-1}, respectively, indicating successful conversion from *p*- to *n*-type behaviour. Using this paint, we found the effect of Adidas Ice Dive perfume remained for 4 hours. The sample exhibits a negative temperature coefficient of resistance of 0.0095 K^{-1} showing the decrease in resistance with temperature. As a result, these films can be easily incorporated into the CMOS fabrication process and employed in bolometers or other IR-detecting equipment materials. This paint can also be used for printed electronic applications, such as batteries, thermoelectric devices, sensors, PCB resistors, etc. Our research reveals that very low resistive electronic circuits and devices can be prepared on flexible paper substrates at an extremely low cost, effortlessly and in a short time duration.

i0037

Improved thermoelectric performance of Yb-filled $CoSb_3$ with the addition of Type-I clathrates

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Yb-Co_4Sb_{12} exhibits a high power factor, making it an excellent material for medium-temperature thermoelectric energy conversion. Type-I clathrates $Ba_8Al_{16}Si_{30}$ (BAS) and optimized Type–I clathrates $(DyBa)_8Al_{16}Si_{30}$ (BDAS) have been added to $Yb_{0.3}Co_4Sb_{12}$ (SKT) to improve its power factor and figure-of-merit. Both materials were vacuum alloyed independently, and hot press procedures were followed to get the resultant materials $(BAS)_x(SKT)_{100-x}$ and $(BDAS)y(SKT)_{100-y}$ with x = 2,4 and y = 1,2 wt.%. A high Seebeck coefficient accompanied by preferable electrical conductivity turns into a high power factor of 3.2 $mW^{-1}K^{-2}$, 25% higher than SKT at 650 K. The power factor started dropping above 650 K due to bipolar conduction. The interfaces between SKT and BDAS are band-matched for both charge transport and phonon transport, as shown by the fact that the thermal conductivity of this composite does not considerably decrease when compared to SKT. At 750 K, the figure-of-merit of the y = 1 wt.% material increases by 20% to a value of about 0.85 compared to 0.7 for SKT.

j) MAGNETISM AND SUPERCONDUCTIVITY

j0001

Metamagnetic Phase Associated with the Quenching of Short-range Magnetic Order in $DyTaO_4$

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Here we report the structural and magnetic investigations on $DyTaO_4$, studied via X-ray diffraction and DC and AC magnetization measurements. $DyTaO_4$ crystallizes in two different space groups i.e., *P*2/*c* (no. – 13, *M'*) and *I*2/*a* (no. – 15, *M*) depending on the annealing conditions. No long-range magnetic ordering and spin freezing is observed down to 1.8 K. However, the presence of broad hump in magnetic susceptibility and deviation from Curie-Weiss law suggest the presence of short-range magnetic ordering. Short range order is more pronounced in *M'* phase as compared to *M* phase. The isothermal magnetization and AC susceptibility analysis uncovers the presence of metamagnetic transitions in both phases, which are believed to arise due to the field induced quenching of short-range magnetic ordering.

j0005

Van-Vleck Contribution to Magnetism and Crystal Field Effects in SmAlGe

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Rare-earth based ternary intermetallics have attracted significant interest in recent years. Here, we report a detailed experimental investigation of physical properties of a ternary intermetallic SmAlGe. Our magnetization and heat capacity studies reveal that an antiferromagnetic ordering is noted around ~ 6.5 K. Interestingly, below 200 K, the temperature dependence of the susceptibility can be fitted by modified Curie-Weiss (CW) law, considering the Van-Vleck contribution from the low-lying first (second) excited multiplet $J = 7/2$ ($J = 9/2$). At higher temperatures, a deviation from CW law is noted which arises due to the low-lying excited energy states. We find that the ground state multiplet splits under the effect of crystal field and levels lie around Δ_1=145.68 K, Δ_2=643.81 K.

j0006

Invar Behavior in Nearly Stoichiometric $TiFe_2$

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The ability of invar materials to maintain its dimensions under varying temperature conditions have provided a means to control the normal thermal expansion. $TiFe_2$ is one such hexagonal Laves phase intermetallic that displays invar like behavior over a wide temperature range. The crystal structure of $TiFe_2$ comprises of antiferromagnetically stacked ferromagnetic Fe 6h planes giving rise to an interesting interplay of magnetic interactions. The strong competition between the in-plane ferromagnetism and out of plane antiferromagnetism is responsible for the observed invar behavior in the nearly stoichiometric $TiFe_2$.

j0007

Exploring 3*d* Transition Metal Substituted $MnCo_{0.7}Fe_{0.3}Ge$

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In this report, we investigate the magnetic properties of MnCoGe by simultaneously yet partially replacing Mn and Co with 3*d*-transition metals. Fe substitution for Co, i.e., $MnCo_{1-x}Fe_xGe$ resulted in the suppression of high temperature martensitic transition and stabilizes the ferromagnetic state around T_C = 250 K for x = 0.3. Partial replacement of Mn by Ni in $MnCo_{0.7}Fe_{0.3}Ge$ i.e., $Mn_{0.7}Ni_{0.3}Co_{0.7}Fe_{0.3}Ge$ is found to crystallize in the hexagonal structure. The temperature dependent magnetization analysis reveals positive Weiss paramagnetic temperature

(indicating ferromagnetic correlations) along with a high temperature paramagnetic to low temperature ferromagnetic transition around 246 K. Decrease of magnetic transition with Ni substitution is attributed to the enhanced antiparallel magnetic interactions of Mn-Ni. Further, the effect of magnetic field on $Mn_{0.7}Ni_{0.3}Co_{0.7}Fe_{0.3}Ge$ will be addressed alongside revelation of universal critical behavior

j0009

Room Temperature Magnetoelectricity in $LiFe_5O_8$

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$LiFe_5O_8$ (LFO) was synthesized by sol-gel auto combustion method. The phase confirmation of the samples was done by the Rietveld refined X-ray diffraction (XRD) patterns. Temperature dependent magnetic properties were investigated by the Vibrating Sample Magnetometer. Temperature dependence of the electrical resistivity suggested polaronic hopping conduction in the high temperature region of 352 - 400 K. The magnetoelectric (ME) measurement revealed the true ME coupling in the sample.

j0010

Spin Compensation in Intermetallic Compound Ho_6Fe_{23}

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Abstract. Compounds exhibiting fascinating phenomenon like spin compensation leading to negative magnetization and anomalous exchange bias have potential for applications in magnetic memories, spin valves, thermomagnetic switches, and spintronics devices. Such phenomenon has been witnessed in several R_6Fe_{23} compounds that crystallize in the cubic (Fm-3m) Th_6Mn_{23} type structure, *R* being the rare earth located at the 24e site and Fe occupying the four distinct positions *viz*. 4b, 24d, $32f_1$, and $32f_2$. In the present work, the structural and magnetic properties of the intermetallic compound Ho_6Fe_{23} that shows magnetization (spin) compensation at ~198 K (T_{comp}) and has an ordering temperature of ~510 K, are studied in a temperature range of 4-575 K. Spin compensation occurs in this compound due to the antiferromagnetic coupling among one Ho and four Fe sub-lattices, as elucidated from our neutron diffraction study. Spin compensation has also been confirmed by neutron depolarization experiment where a complete recovery of the neutron beam polarization occurs near the T_{comp} (198 K). DC magnetization, neutron depolarization, and neutron diffraction techniques are employed to establish an in-depth understanding of negative magnetization at the macroscopic, mesoscopic, and microscopic levels, respectively.

j0011

Growth And Structural Characterization Of Fe_xSe_{1-x} Thin Films: Exploring Its Critical Temperature Tunability With Varying Thickness

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FeSe thin films were deposited on CaF_2 substrates via pulsed laser deposition to investigate their superconducting properties. Structural characterization using X-ray diffraction (XRD) confirmed the films' tetragonal phase, while scanning electron microscopy (SEM) revealed the presence of small iron-rich precipitates on the film surface, resulting in an overall composition of 0.6:0.4 of Fe:Se. Thickness-dependent measurements of the superconducting transition temperature (T_c) were conducted, showing that T_c decreases with decreasing film thicknesses with films below 33 nm becoming non-superconducting. Formation of CaSe dead interfacial layer might lead to this observed variation.

j0014

Enhanced Magnetic And Magnetodielectric Coupling In 0.5 ($Bi_2Fe_4O_9$)-0.5 ($La_{0.67}Sr_{0.33}MnO_3$) Composite

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In the present work, we have discussed the magnetic and magnetodielectric effect in 0.5 ($Bi_2Fe_4O_9$)-0.5 ($La_{0.67}Sr_{0.33}MnO_3$) composite. Rietveld refinement of XRD data shows phase purity of the composite revealing its dual phase orthorhombic structure. Enhanced magnetization along with weak ferromagnetism is evidenced from temperature dependent magnetization (M-T) data and isothermal magnetization (M-H) plots. Irreversibility in ZFC-FCW is seen around 340 K suggesting spin glass behavior. Two magnetic transitions i.e. $T_I \sim 300$ K and $T_{II} \sim 65$ K is seen which matches well with anomalies in temperature dependent dielectric study, thus indicating MD coupling in the composite which was further ascertained from field dependent MD% study at the higher frequency range. Lastly, from Ginzburg-Landau free energy theory, the absolute value of coupling coefficient (γ) is determined to be 0.022 $(emu/g)^{-2}$ at 300 K which implicates that MD effect emerges from the coupling term *'γP^2M^2'*. Hence, above striking properties make this material a sustainable candidate for multifunctional device applications.

j0015

Study of Electrical Resistivity of Fe-Based Superconducting Compounds

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The resistivity of Fe-Based superconductor (LaFeAs) was analyzed theoretically, with a focus on its temperature dependence. The resistivity was analyzed using the electron-phonon model, specifically the Bloch-Gruneisen model. We derived the Debye temperature and Einstein temperature from an overlap repulsive potential, it was found that optical phonons have a greater impact on resistivity than acoustic phonons at certain higher temperatures while acoustic phonons dominate below that temperature. By considering acoustic and optical phonons with zero limited resistivity, the total resistivity was calculated which shoes a quadratic temperature dependence. The contribution of electron-electron inelastic scattering was found by dependence of $\rho_{diff.} = [\ \rho_{exp} - \{\rho_0 + \rho_{e\text{-}ph}\ (= \rho_{ac} + \rho_{op})\}]$. The analysis supports the use of the BG electron-phonon model for this system. Kresin's strong coupling theory was used to calculate the superconducting transition temperature and isotope effect exponent, which suggest that the electron-phonon interaction is an important factor in the pairing mechanism.

j0016

Study of Strongly Correlated Electron System CeM_2Al$_8$ (M = Fe, Co)

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The magnetic f- and d-electron elements in which hybridization with conduction electrons results in enhanced densities of states close to the Fermi energy beget a wealth of physical phenomena. In the present work, we have undertaken the study of two isostructural compounds, CeM2Al8, with a difference of one electron between the two transition metals (M = Fe and Co). However, irrespective of this small change in the electron count, and a variation in the unit cell parameters, it is found that the Fe compound exhibits mixed valence of Ce where the Co compound exhibits full free ion magnetic moment of Ce. The study of both the compounds implies varying degrees of electronic correlational phenomena.

j0017

First-Principles Investigation of FeSb2 as a Novel Altermagnetic Material

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This work explores the influence of altermagnetism (AM) on the electronic structure of materials, specifically focusing on the emergence of non-relativistic spin splitting [1]. We demonstrate that the k-path dependence of altermagnetic spin splitting in the 3D Brillouin zone exhibits distinct altermagnetic surface states due to specific surface orientations. By considering orthorhombic space groups we unveil the altermagnetic properties of the surface states. We calculated the 2D projected Brillouin zones from the bulk and analyzed the interaction between these surface Brillouin zones and

the k-dependent spin splitting. This analysis identifies surfaces where opposite-sign spin splitting merges, nullifying altermagnetism and surfaces where altermagnetism is preserved. Our investigation across the three principal surface orientations reveals that for several cases, two surfaces exhibit "blindness" to the altermagnetism, while the remaining surface retains altermagnetic properties [2]. This dependence on surface orientation is further influenced by the specific magnetic order within the material. Therefore, our work provides a framework for understanding and tailoring surface AM, paving the way for potential applications in spintronics and related fields.

j0018

Multiferroic order in Gd2MnFeO6: Significance of magnetic frustration

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We present a noteworthy finding of high-temperature ferroelectric order in a fairly unexplored Gd2MnFeO6 compound, characterized by a disordered double-perovskite structure. This material exhibits a remarkable cryogenic refrigerant capacity alongside the ferroelectric order, making it a rare occurrence. Notably, the refrigerant capacity of this Gd-based double perovskite surpasses that of all previously reported counterparts. Around 92 K (T_{FE}), we observe the presence of ferroelectric order, which is significantly higher in temperature compared to the magnetic order at 4 K (T_N). The involvement of dominant short-range magnetic order below T_{FE}($>>T_N$) leads to a notable magnetoelectric consequence The high-temperature ferroelectric order associated with the linear magnetoelectric coupling is in tune with the strong magnetic frustration in Gd2MnFeO6.

j0019

$NiBi_3$ Nanowire-Based Planar Nano Josephson Junctions via Ion Implantation

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Josephson junctions are superconducting devices where two superconductors are separated by a thin, non-superconducting barrier, leading to a characteristic current-phase relationship ($I = I_0 \sin \Phi$). Fabrication techniques like planar and vertical geometries, or Dayem bridges, influence junction properties. The weak link's dimensions are crucial for optimal device performance. We explored creating planar nanowire Josephson junctions from $NiBi_3$ nanowires using Ga-ion irradiation. This is particularly interesting because $NiBi_3$ exhibits a strong resistive state, leading to highly resistive electrodes in the resulting junctions – a departure from conventional Josephson junctions. While the irradiated nanowires displayed I-V curves resembling Josephson junctions with very low critical currents, a definitive indicator is the presence of Fraunhofer patterns. These patterns manifest as oscillations in the critical current versus applied magnetic field ($\mu_0 H$) or voltage across the junction (V) at a fixed current bias. Our V-H curves indeed exhibited Fraunhofer-like oscillations with a background magnetoresistance of the nanowire. The extracted flux quantum from this quantization was 2.24×10^{-15} Wb·m², very close to the expected value.

j0020

Glassy Magnetic State and Carrier localization Effect in *β*-Mn Type $Co_7Zn_7Mn_6$ and $Co_7NiZn_7Mn_6$ Alloys

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Co-Zn-Mn alloys with β-Mn-type structure are an important new member of the skyrmion-hosting chiral magnets. The remarkable characteristic of these materials is the stable formation of skyrmions above room temperature, which is essential for realizing skyrmion-based devices. Here, we investigate the magnetic and transport properties of two such compounds: $Co_7Zn_7Mn_6$ and Ni-doped $Co_6NiZn_7Mn_6$. Both of these alloys crystallize in a β-Mn type chiral cubic structure with space group $P4_132$. The parent compound $Co_7Zn_7Mn_6$ shows a paramagnetic to ferromagnetic transition at around 195 K, while the Ni-doped sample shows the transition around 123 K. Both samples exhibit a glassy magnetic state. The memory measurement indicates that Ni-doping enhances the glassy nature of the parent sample. Interestingly, both alloys show a carrier localization effect in the longitudinal resistivity (ρ_{xx}) at low temperatures. For both compounds, the ρ_{xx} shows a $T^{1/2}$-like dependence at low temperatures, which originates from the electron-electron

interaction effect. Ni-doping introduces more disorder, as the localization effect is more pronounced in the Ni-doped sample.

j0021

Investigating the Magnetocaloric Effect and Glass Forming Ability of $Fe_{86-2x}Zr_{8+x}B_{5+x}Cu_1$ Metallic Glass Ribbons

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The magnetocaloric effect (MCE) and glass forming ability (GFA) of quaternary metallic glass (MG) amorphous $Fe_{86-2x}Zr_{8+x}B_{5+x}Cu_1$ (x=0,1& 2) ribbons were comprehensively examined in this study. Rapid solidification formed the metallic glasses into a ribbon with typical amorphous properties. XRD, DSC, TEM, and VSM characterisations analysed their structure and magnetic properties. The ribbons' glass-forming ability (GFA) was calculated using thermodynamic parameters. The magnetization-temperature graph reveals that boron and zirconium raise the Curie temperature and shift entropy from 1.68 to 2.01 J/KgK at 2.5 T. Additionally, it exhibits a noteworthy relative Cooling Power of 38.76-53.74 J/Kg. The potential of this material as an exceptional low-temperature refrigeration material around room temperature is demonstrated by these outcomes.

j0022

Rigid and Flexible BZT-YIG Composite for Energy Conversion and Shielding Application

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Multiferroics are now in the front of cutting-edge research because to their unique properties and potential applications in advanced technology. This research delves into two possible applications of multiferroics: one for magnetoelectric (ME) energy harvesting using rigid materials, and the other for electromagnetic interference shielding using flexible materials. The study of rigid multiferroics, (($Ba_{0.5}Zr_{0.5}TiO_3$ (BZT) + $Y_3Fe_5O_{12}$ (YIG)) (BY)), is being conducted for utilisation in ME applications. An optimised microstructure and material composition of a rigid BY composite resulted in an enhanced ME coupling coefficient of 1.74 mV/(cm-Oe). As the use of ME harvesters with AI continues to grow, a new form of pollution called electromagnetic interference has surfaced. This calls for materials that can withstand electromagnetic radiation while yet being pliable. For this reason, we tested PVDF/BY (PBY) flexible films with 10, 20, 30, and 40 wt.% ceramic to see how well they blocked electromagnetic interference. A reflection loss of −47.9 dB is observed, indicating that the PBY composite with 40 wt% offered outstanding absorption capability.

j0023

Optimization of growth of superconducting Nb_3Sn films with varying thickness

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In this study, we investigate the growth and characterization of niobium-tin (Nb_3Sn) thin films and analyze the variation in their superconducting transition temperature (T_c) with respect to film thickness. Nb_3Sn films of varying thicknesses from 1000 – 8 nm were deposited using DC magnetron sputtering on silicon and magnesium oxide substrates. Growth conditions were optimized which gave a T_c of 17.8 K for the thickest film. The films were characterized using X-ray diffraction (XRD) and scanning electron microscopy (SEM). Nb_3Sn A15 phase was seen to form in films down to the lowest thickness. Homogenous, films with Nb:Sn ratio of 3:1 was obtained for all the films. Besides, the films were nanocrystalline with the grain size ranging between 40 – 20 nm. T_c was observed to decrease with decreasing film thickness. This variation can be attributed to the increase in disorder originating from the decrease in particle size with decreasing thickness in these Nb_3Sn nanocrystalline films. Thus, our studies show that Nb_3Sn thin films form a good model system to explore the role of disorder on the superconducting properties.

j0024

Magnetic Interactions in Spin-Orbit Entangled $4d^3$ Oxide Ca_3LiRuO_6

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Magnetic interactions play an important role in determining the magnetic ground state and thermodynamic properties of a material. Here, we have calculated the exchange interaction in a 4*d* transition metal oxide compound Ca_3LiRuO_6 , using the magnetic force theory (MFT).To determine the exchange interactions, the maximally localized Wannier functions, calculated using WANNIER90 were used. The obtained magnetic exchange interaction constants (*J*) show excellent agreement with inelastic neutron scattering data.

j0025

First-Principles Study Of The Electronic Structure And Magnetism In Highly Frustrated Two-Dimensional Magnet $CsTbSe_2$

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Rare-earth compounds with spins arranged in a frustrated triangular lattice are extremely exotic for unconventional ground state properties. In this context various rare-earth based systems such as $YbMgGaO_4$, $CsNdSe_2$ and $TbInO_3$ have been predicted theoretically as well as experimentally belonging to a class of spin-liquid materials. Motivated by such exotic ground state properties we have theoretically studied the electronic and magnetic properties of less explored Rare-earth based material namely, $CsTbSe_2$, where Tb ions are arranged in a triangular geometry with two dimensional (2D) hexagonal layers. We employed density functional theory + Hubbard U approach including the effects of spin- orbit coupling (SOC) to understand the ground state electronic and magnetic properties in detail. Our electronic structure calculation reveal that $CsTbSe_2$ is a SOC driven insulator with a gap of 1.80 eV. To understand the magnetic properties, we calculated the exchange coupling strength for various neighbors and found that Tb ions are arranged in frustrated triangular antiferromagnetic arrangement with negligible interaction between the Tb-hexagonal layer along the c-axis. Hence, our findings reveal that this material is a highly frustrated two-dimensional (2D) magnet with insulating ground state and can be a promising candidate for antiferromagnetic spin-liquid or can host incommensurate magnetic structures.

j0026

Large Dielectric Constant In Metamagnetic Eu_2CoMnO_6

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We report on the electrical and magnetic properties of polycrystalline Eu_2CoMnO_6. The X-ray absorption spectroscopy shows the mixed valance states of Co/Mn cations. The resistivity measurement shows the semiconducting nature of Eu_2CoMnO_6. 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.

j0028

Investigation of Magnetic Ordering and Exchange Bias in Double Perovskite, Ho_2CoMnO_6

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We have investigated magnetic ordering and exchange bias (EB) phenomenon in double perovskite, Ho_2CoMnO_6 (HCMO). The HCMO compound crystalizes in *P21/n* space group as confirmed by x-ray diffraction and neutron powder diffraction (NPD) study at room temperature. The dc magnetization (*M*) vs. temperature (*T*) curve under 100 Oe increases sharply below 85 K suggesting a ferromagnetic type ordering below the critical temperature (T_C) of ≈ 75 K. This finding is corroborated by temperature dependent NPD study that infers a ferromagnetic ordering between Co^{2+} and Mn^{4+} moments below 75 K, whereas Ho^{3+} remains paramagnetic down to 5 K. The magnetic moments of

Co^{2+} and Mn^{4+} are aligned in [10$\bar{1}$] crystallographic direction. The magnetic isotherms (*M* vs. *H* curves) reveal the presence of negative EB in the sample. The EB field peaks at 5 K and decreases with increasing temperature, disappearing completely above 20 K. The observed EB in HCMO is explained in the framework of antiparallel polarization of Ho^{3+} moments under the influence of the internal field from the ferromagnetic alignment of Co^{2+} and Mn^{4+} moments. Additionally, coercivity and remnant magnetization values derived from *M*(*H*) curves peak around 10 K and exhibit a non-monotonous behaviour below 10 K. This complex magnetic behaviour of HCMO is investigated by employing dc magnetization, neutron diffraction, and neutron depolarization techniques.

j0030

Effect of Ni-substitution in M-type Hexaferrites $SrNi_xFe_{12-x}O_{19}$: A Mössbauer Study

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The $SrNi_xFe_{12-x}O_{19}$ (where x = 0.0 - 1.0 in steps of 0.2 wt%) were synthesized using Co-precipitation method. The powders were sintered for 4h at 1100 °C using conventional sintering method. The structural, morphological, hyperfine interactions properties were investigated at room temperature. The lattice parameters 'a' & 'c' increased with *x*. The shape of the grains was hexagonal in nature and the average grain size found to be decreased with Ni^{2+} doping. The value of average grain size (<D>) was found between 1.713m ($x = 0$) - 0.549m ($x = 1.0$). Mössbauer study indicates that Ni^{2+} ions preferentially occupy 2*a* and 4f_2 sites up to $x = 0.6$ beyond $x > 0.6$, Ni^{2+} ions occupy 12*k* and 4f_2 sites. There is a paramagnetic contribution (0.7 – 2.7%) up to $x = 0.6$ composition which is reduced with increasing the Ni^{2+} ions. All Fe-ions were found in Fe^{3+} high spin states.

j0033

Role of Magnetic field on Electronic Specific Heat of Anderson Lattice Model: An Application to Colossal Magnetoresistive Manganites ($Re_{1-x}A_xMnO_3$)

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We have studied the role of magnetic field on electronic specific heat (C_v) at different temperatures of rare earth manganites doped with alkaline earths namely $Re_{1-x}A_xMnO_3$ (where Re = La, Pr, Nd etc., and A= Ca, Sr, Ba etc.) exhibiting colossal magnetoresistance (CMR) phenomena. We have used a two band (l-b) Anderson lattice model Hamiltonian to study these materials in the strong electron-lattice Jahn- Teller (JT) coupling regime an approach similar to the two- fluid models. We find that linear coefficient of specific heat C_v / T increases with increasing magnetic field 'h'& 'm' parameters showing the peak at low temperatures & finally decreases at higher values of h, m parameters. We have plotted the curves at temperature 100 K & 300 K only. We have also observed the role of doping concentration 'x' on specific heat coefficient (C_v /T). It increases with the doping 'x' having the peak near x=0.3 which shows the optimum value of x and decreases thereafter on higher values of x. Our results are in good agreement with the available experimental data.

j0034

Cluster Spin Glass Behavior in Co (II) Based Supramolecular Metallogel

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Supramolecular metallogels, an attractive field in the hybrid inorganic-organic materials family, are a class of gels created through the arrangement of low molecular weight organic components. Magnetism in Supramolecular metallogels is driven by the cooperative exchange interaction between metal centers mediated through the bridging

ligands. Therefore, magnetic behavior depends on the intrinsic nature of the paramagnetic metal ions, organic ligands and the topology of the compound. Here, we report the magnetic properties of a cobalt-based supramolecular metallogel, Co(II)-3-amino-1-propanol, forming a chain-like structure of Colat octahedra connected through organic ligands. From the analysis of dc magnetization, which shows bifurcation between FC and ZFC curves and a cusp in ZFC, it is inferred that the system undergoes a transition from paramagnetic to a spin-glass like state below 20 K. Analysis of the dc and ac magnetization measurement results employing various models such as Vogel-Fulcher, Power law and anisotropic Heisenberg chain model indicates that the competing ferromagnetic intrachain and antiferromagnetic interchain interactions lead to Cluster-Spin-Glass behavior in systems.

j0036

Green Synthesis and Characterization of Sugar-Coated Superparamagnetic $Zn_{0.5}Co_{0.5}Fe_{1.8}M_{0.2}O_4$ and $Zn_{0.5}Co_{0.5}M_{0.2}Fe_2O_4$ (M = Mg and Ca) Magnetic Dotes

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In the current era of nano-miniaturization, magnetic dots (MDs) are catching attention for their potential biomedical applications like magnetic hyperthermia-mediated cancer therapy (MHCT) and contrast agents. These MDs need to be surface functionalized and biocompatible for which green synthesis is a simple one-step solution. Sugarcane juice-mediated MDs can be a double-edged sword for MHCT: targeting cancer cells by localized heat transfer along with cytotoxic potential against cancer cells due to organic moieties like polyphenols attached to the surface. This work reports structural and magnetic properties of four nanoferrites viz; $Zn_{0.5}Co_{0.5}Fe_{1.8}Mg_{0.2}O_4$ (ZCFM), $Zn_{0.5}Co_{0.5}Fe_{1.8}Ca_{0.2}O_4$ (ZCFC), $Zn_{0.4}Co_{0.4}Mg_{0.2}Fe_2O_4$ (ZCMF) and $Zn_{0.4}Co_{0.4}Ca_{0.2}Fe_2O_4$ (ZCCF) synthesized by sugarcane juice mediated sol-gel tactics. Rietveld, Raman, FTIR, and HRTEM analysis affirmed formation of surface functionalized MDs with a mean particle size in the range 4 to 7 nm. These MDs exhibited superparamagnetic (SPM) character at 300 K, which is well corroborated by modified Langevin function fitting. Overall, sugarcane juice as green fuel in the self-combustion tactics proven to be simplest route for the fabrication of sugarcoated SPM with better magnetic characteristics.

j0037

Green Synthesis of Spinel Nanoferrites: Integrating Size Control, Superparamagnetism and Surface Functionalization

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Tailoring structural and magnetic properties of spinel nanoferrites (NFs) with effective control over their particle size and infusing biocompatibility is a central theme for magnetic hyperthermia-mediated cancer therapy . Here, we report successful use of sugarcane juice as a promising bio surfactant to control the magnetic properties of phase pure spinel NFs viz. $ZnFe_2O_4$ (ZFO), $Zn_{0.7}Ca_{0.}15Mg0_{.15}Fe_2O_4$ (ZCMFO), $Zn_{0.35}Co_{0.35}Ca_{0.15}Mg_{0.15}Fe_2O_4$ (ZCCMFO) and $Co_{0.7}Ca_{0.15}Mg_{0.15}Fe_2O_4$ (CCMFO), $CoFe_2O_4$ (CFO). PXRD, Raman, FTIR, TGA, XPS and HRTEM analysis revealed the formation of poly dispersed samples with functionalized surfaces with mean particle size in the magnetic quantum dot regime (4-11 nm). ZFO, ZCMFO, ZCCMFO and CCMFO exhibited SPM character at 300 K which is well corroborated by modified Langevin function fitting, while CFO is as an assembly of SPM and FiM at 300 K. Overall, green synthesis infused critical control of particle size, tuned magnetic hardness, imparted SPM character & surface coating without compromising magnetization is indeed remarkable.

j0039

Structural And Magnetic Properties Of The Cluster-Glass Phase Of Pseudo -1-D Spin-Chain Compound $Ca_3Co_2O_6$

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Abstract: We investigated the structural and magnetic characteristics of $Ca_3Co_2O_6$ using powder X-ray diffraction (XRD) and magnetization measurements. The quasi-one-dimensional spin chain compound $Ca_3Co_2O_6$ was synthesized via the solid-state reaction method. The sample was characterized using room temperature XRD and magnetic measurements. Rietveld refinement of the XRD data indicates that the sample crystallizes in a rhombohedral

phase with space group $R\bar{3}c$. The material undergoes a phase transition from a paramagnetic phase to a disordered antiferromagnetic phase below 25 K (T_{C1}), and a glassy phase appears below 11.20 K (T_{C2}). The magnetization measurements taken with a wait period showed a reduced saturation moment of 0.2 μ_B/f.u. at 9T magnetic field. Additionally, interrupted field cool cooling (IFCC) magnetization measurements demonstrated a magnetic memory effect below the glassy temperature.

j0040

Investigation into Microstructural Evolution and Magnetic Behavior of As-Cast Co-rich Zr Alloys

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Abstract: In this study, the as-cast microstructures and magnetic properties of Co-rich Zr alloys, Co–x at.% Zr (x = 13, 15, 17), have been investigated. The microstructural evolution in these alloys was analysed using X-ray diffraction and scanning electron microscopy techniques. It was observed that the microstructural featureSSPSs of these alloys, in their as-cast condition, vary significantly with increase in the Zr content. The room temperature magnetization behaviour of the as-cast alloys revealed a decrease in magnetization with increase in the Zr content. The change in magnetic properties has been rationalized with the observed microstructural changes.

j0041

Structural and Magnetic Studies of Doped $BiFeO_3$

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In this paper, we report the synthesis of $BiFeO_3$ and the effects of doping on its structural and magnetic properties. Lanthanum was substituted for bismuth, and transition metals (Co, Mn, and Ni) were substituted at the iron lattice sites. Undoped and doped $BiFeO_3$ powder samples were prepared using an eco-friendly citrate combustion method. It was observed that doping aids in phase stabilization, as confirmed by the XRD patterns. While undoped $BiFeO_3$ exhibited paramagnetic behavior at room temperature, it transformed into a ferromagnetic state upon transition metal doping. The Neel temperature increased with cobalt (750K) and nickel(650K) doping, whereas it decreased with manganese doping(630K) due to changes in the magnetic interactions at the B-sites in the perovskite ABO_3 structure of $BiFeO_3$.

j0042

Investigation of 160 MeV Ni^{12+} Ion Induced Alteration in Magnetic Properties of Mn-Co Ferrite Nanoparticles

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Irradiation with swift heavy ions (SHI) is a noval way to alter distribution of cations and hence characteristic properties of spinel ferrites. Present investigation showed the effect of 160 MeV Ni^{12+} ion irradiation on magnetic properties of $Mn_{0.25}Co_{0.75}Fe_2O_4$ (MCF) nanoparticles (NPs). MCF NPs were synthesized through citric acid-assisted sol-gel auto-combustion method and annealed at 400 ^{0}C. The synthesized NPs were irradiated with two ion fluences of 5×10^{12} and 1×10^{13} ions/cm^2. Different analytical techniques such as X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy and vibrating sample magnetometer (VSM) were used to analyze the structural phase, chemical composition and magnetic characteristics of pristine as well as irradiated MCF NPs. Pristine as well as irradiated NPs exhibited characteristic reflection planes corresponding to cubic closed packed (fcc) spinel phase. Two significant broad adsorption bands in FTIR spectra were clearly observed for all the NPs which confirmed the retention of spinel phase of MCF NPs after Ni^{12+} ion irradiation. VSM analysis showed that all NPs exhibited ferrimagnetic hysteresis loop of MCF NPs at 20K and 300K. However, asymmetry was observed in the hysteresis loop of MCF@5E12 NPs measured at 20K. This was attributed to induced permanent magnetization after irradiation. This could to be helpful for permanent magnet application in electronic industries. The saturation was not achieved in magnetization even at external field of strength 1.8 kOe. This was because of higher magneto-crystalline anisotropy of parent cobalt ferrite

NPs. Thus, the "law of approach" was used to determine magneto-crystalline anisotropy constant (K) and saturation magnetization (M_S) of pristine and Ni^{12+} ion irradiated MCF NPs. Significant variations were observed in different magnetic characteristics MCF NPs. Therefore, Ni^{12+} ion irradiation is a potential way to tune the magnetic characteristics of spinel ferrite nanoparticles as per demand of specific application.

j0043

Edge States for a Ribbon Oriented in the Diagonal Direction in 2D Antiferromagnetically Ordered Semimetals

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We explore the nature of edge states in a 2D topological semimetallic state with antiferromagnetic (AFM) ordering in the presence of nearest-neighbor (NN) Rashba spin-orbit coupling (SOC). For this, we adopt a ribbon geometry, different from the conventional arrangement of horizontal or vertical, extended collinearly with the AFM ordering direction such that the basis atoms belonging to the same sublattice lie on one chain which alternates in between the chains of different sublattices. With this choice of ribbon orientation, we found that the edge state dispersion gaps in the magnetically ordered state, in contrast to the flat bands as obtained with the conventional choice of ribbon geometry. Our findings underscore the influence of ribbon orientation relative to the magnetic ordering direction on the nature of these edge states.

j0045

Polymorphism in $NdIr_3$

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$NdIr_3$ crystallizes in two cubic polymorphic structures ($AuCu_3$- and $AuBe_5$-type) that coexist together macroscopically. Interestingly, the magnetic behavior of these two cubic phases is quite contrasting: one exhibits ferromagnetic ordering, while the other remains paramagnetic down to 2 K. Determining the magnetic and physical characteristics of a compound with coexisting polymorphic phases is quite challenging. If these polymorphs exhibit identical magnetic ordering, understanding the magnetic interaction and its relationship with magnetic atoms becomes even more daunting, particularly requiring magnetic isotherms near the magnetic ordering. The presence of multiple magnetically ordered phases in the compound results in complex magnetic isotherms characterized by a dynamically changing slope at the onset of domain rotation. As the $AuCu_3$-type polymorph of $NdIr_3$ does not display magnetic ordering, it presents a unique opportunity to thoroughly investigate the magnetic interactions of the ferromagnetic $AuBe_5$-type phase. In our study, we utilized magnetic isotherms and specific heat to estimate critical exponents, which are crucial parameters for identifying the magnetic universal class.

j0046

Structure, Morphology and Magnetic Properties of $TmCrO_3$

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Abstract: The structure, morphology, and magnetic properties of $TmCrO_3$ are presented here. The crystal structure and phase purity of the sample were confirmed by Rietveld refinement of X-ray and neutron powder diffraction data. Scanning electron microscopy (SEM) and energy dispersive analysis of X-ray (EDAX) have been employed to study grain morphology, compositional homogeneity and elemental composition. Temperature dependent DC magnetization measurement revealed an antiferromagnetic transition at 125 K and a spin reorientation transition below 5 K, accompanied by negative magnetization, confirming the anticipated magnetic behavior of $TmCrO_3$.

j0047

Tunable Magnetism in Manganese Ferrite Nanoparticles Under Vacuum and Air Annealing

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Manganese ferrite (MFO, $MnFe_2O_4$) nanoparticles are prepared by co-precipitation method. The as prepared MFO nanoparticles are annealed in vacuum and air atmosphere at 1000℃ for two hours separately. The XRD analysis confirms the spinel structure of MFO nanoparticles for both pristine and vacuum annealed ones, whereas upon air annealing the spinel MFO is converted into non-magnetic hematite phase. However, when re-annealed in vacuum the air annealed sample converted back into spinel structure. These structural changes under different annealing conditions corroborate with the room temperature magnetic measurements. The M vs H loops are obtained for the pristine MFO, and vacuum annealed MFO shows a large M_s value of 50.41 and 59.97 emu/g with low H_c value of 35.0 and 41.06 Oe respectively. Due to the presence of non-magnetic phase upon air annealing the M_s of MFO is drastically dropped to 2 emu/g with a large coercive field H_c about 204.5 Oe.

j0048

Studies of the Electrical and Magnetic Properties of Frustrated Spinel $Mg_{0.5}Mn_{0.5}Cr_2O_4$

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In the present case, we have tried to explain the structural, magnetic, and electrical properties of the $Mg_{0.5}Mn_{0.5}Cr_2O_4$ spinal ceramic compound. We have prepared the ceramic compound using the solid-state reaction method. The room temperature XRD is used to check the phase purity of the sample. Rietveld refinement methods are used from the XRD data to understand the structural parameters. The Rietveld refinement of the $Mg_{0.5}Mn_{0.5}Cr_2O_4$ sample confirmed a single-phase cubic spinel structure with space group Fd-3m. The electrical and magnetic properties of the spinel ceramic compound are studied using an LCR meter and physical properties measurement system (PPMS)-VSM. Our study aims to investigate the electrical and magnetic properties of the $Mg_{0.5}Mn_{0.5}Cr_2O_4$ ceramic compounds. Here, we have tried to explain the nature of the frustrated $Mg_{0.5}Mn_{0.5}Cr_2O_4$ ceramic compounds. Temperature and field-dependent magnetic properties are used to understand the magnetic behaviors of the sample deeply.

j0049

Structural and Magnetic properties in Bi3+ substituted Strontium Hexaferrite

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A detail study of structural, magnetic and microwave properties of Bi^{3+} substituted strontium hexaferrite is carried out explicitly. The desired samples, $Sr_{1-x}Bi_xFe_{12}O_{19}$ (x = 0 and 0.015) are prepared using ethylene glycol and citric acid assisted sol-gel auto-combustion method. Different characterization techniques such as XRD, SEM, magnetic measurements are adopted to analyze the various physical properties due to substitutions. Rietveld refinement of XRD data confirms that, the prepared samples crystallize in hexagonal structure belonging to $P6_3/mmc$ space group. With substitutions, saturation magnetization (M_s) decreases and coercivity (H_c) increases as compared to the parent one.

j0050

Large Magneto-caloric Effect near Room Temperature in $Ni_{37}Co_{13}Mn_{34}Ti_{16}$ alloy

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We report a large magneto-caloric effect in $Ni_{37}Co_{13}Mn_{34}Ti_{16}$ alloy near room temperature across the magnetostructural transition. A maximum entropy change of nearly 8.6 $Jkg^{-1}K^{-1}$ was observed near 307 K for a magnetic field change of 70 kOe. We also observed the effect of heat treatment on the sample.

j0054

Atomic Scale Study of Defects in Si substituted Co_2FeAl Heusler Compounds

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Full heusler compound Co2FeAl composed of Co and Fe having high values of magnetic moments is reported to exhibit spin polarization close to only 58% against the theoretical prediction of half metallicity. This study addresses the role of lattice disorder in Co2FeAl and its evolution with respect to electron doping by means of substitution of Si at Al sites affecting the lattice ordering/ disordering at atomic scale using Mössbauer spectroscopy.

j0055

Inducing vacancy to alter the magnetic structure of magnetic equiatomic alloy MnNiGe

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Off-stoichiometric alloy of composition $MnNi_{0.9}Co_{0.1}Ge_{1.05}$ is explored through structural and magnetic analysis. In-situ synchrotron X-ray diffraction clearly shows a martensitic phase transition (MPT) from hexagonal to orthorhombic structure, but the transition is incomplete and a significant amount of high-temperature (*T*) phase is found at low-*T*. Magnetic investigations imply that the crystal undergoes a paramagnetic to commensurate antiferromagnetic (AFM) structure in the austenite phase and another magnetic transition coupled with MPT is from commensurate AFM in the austenite phase to incommensurate AFM in martensite phase when cooled from room *T*. At high applied magnetic fields, a magnetic field-induced transition is observed. The alloy shows both inverse and conventional magnetocaloric effect.

j0056

Beyond ferromagnetic resonance: Effect of inertia tensor on dynamic susceptibility

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Ultrafast manipulation of magnetic order with magnetic inertia provides an opportunity for advancement of the data storage devices. Several theoretical studies on magnetic inertia have considered inertia as a scaler quantity. Here we investigate the effect of tensorial inertia on the dynamic susceptibility for ferromagnets, as recent works suggest inertia to be a tensor. We found the inertial susceptibility response at THz frequency along with the traditional ferromagnetic resonance at GHz. Their sense of rotation are opposite to each other.

j0058

Unusual Magnetic and Large Magnetocaloric Behavior of RGa_2 (R = Gd, Tb, Dy, and Ho) alloys

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X-ray powder diffraction and DC magnetization studies have been carried out in the temperature range of 2–300 K for the rare-earth-based antiferromagnetic RGa_2(R=rare-earth elements: Gd, Tb, Dy, and Ho) compounds. The alloys are found to crystallize in a hexagonal (space group: P_6/mmm) structure at room temperature. RGa_2 (Gd, Tb, Dy, and Ho) compounds order antiferromagnetically at T_N (23, 19 , 12 and 9 K respectively). In addition to the primary antiferromagnetic ordering, the DC magnetization data reveals the presence of large thermal hysteresis in zero-field-cooled & field-cooled data and multiple spin reorientation transitions within the antiferromagnetic phase, indicative of a rich variety of magnetic sub-phases. The isothermal magnetization measurements further corroborate these findings, indicating the alloys have very complex magnetic structures. The observed low crystalline electric field effects in $GdGa_2$ alloys can indeed be attributed to the nature of the Gd^{3+} ion as an S-state ion. The existence of a very large conventional magneto-caloric effect (ΔS = -2.7, -4.5, -13.4, and -26.4 J/kg-K for ΔH =80 kOe for RGa_2 (R = Gd, Tb, Dy, Ho) alloys respectively) is another crucial outcome of our study.

j0060

Effect of Off-Stoichiometry on Structural, Electrical Transport, and Magnetic Properties of CrSb

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Among 3d transition metal (TM) mono-antimonides, CrSb stands out as a promising candidate for spintronic applications at room temperature due to its antiferromagnetic structure with perpendicular magnetic anisotropy and high Néel temperature (T_N ≈710K). However, the synthesis of these binary 3d TM mono antimonides is quite challenging as they commonly form off-stoichiometric hexagonal NiAs-type structure with vacancy-defects. Such $TM_{1\pm x}Sb$ off-stoichiometry plays a crucial role in determining the electrical transport, magnetic properties, and carrier concentration of these compounds. Herein we report on the physical properties of a series of $Cr_{1\pm x}Sb$ compositions. These compositions were synthesized using solid state method and characterized for its crystal structure and phase purity using X-ray diffraction (XRD). The local structure of these off-stoichiometric compositions has been studied using Extended X-ray absorption fine structure (EXAFS). The electrical transport was measured in the temperature range of 20 – 300 K and effect of excess Cr in $Cr_{1+x}Sb$ compositions is discussed.

j0063

Novel Synthesis Of $Cuseo_3.2H_2O$: Structural And Magnetic Characterizations

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Here, we report a novel cost-effective, energy-efficient room temperature technique for synthesizing single crystals of $CuSeO_3.2H_2O$ using a single diffusion gel technique with a crystallization period of 14 days. The single crystallinity and the phase purity of the sample were confirmed through both single crystal and powder X-ray diffraction (P-XRD) techniques. P-XRD confirms the orthorhombic $P2_12_12_1$ structure for the crystals. EDAX suggested the formation of $CuSeO_3.2H_2O$ with expected elemental composition. To explore the magnetic properties, DC magnetization of the polycrystalline samples was done in both ZFC and FC modes. $CuSeO_3.2H_2O$ is an antiferromagnet with Néel transition, T_N = 26.7 K, and shows a paramagnetic behavior above T_N, obeying Curies-Weiss law with a Curies temperature of - 92.6 K. The isothermal magnetization studies suggest a metamagnetic spin-flop transition in the system. The field at which the spin-flop transition happens decreases with an increase in temperature.

j0064

Low Temperature Glass–Like Arrestation Formed by Kinetic Arrest of First Order Phase Transition

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A first order phase transition of half doped $Nd_{0.5}Sr_{0.5}MnO_3$ (NSMO) manganite exhibiting hysteretic temperature dependance behavior of magnetization as well as resistivity at nanoscale and doping effects are yet to be studied. By keeping this in mind, NSMO sample was prepared by sol–gel method and sintered at high temperature (~ 1250 °C) to get nearly perfect crystalline structure. The sample NSMO was characterized by X–ray diffraction (XRD). A systematic investigation of magnetization was carried out to understand the magnetic behavior of NSMO. A comprehensive investigation of the ferromagnetic metallic (FMM) to antiferromagnetic insulator (AFI) transition from low temperature has been realized for NSMO. The sample shows anomalies across the AFI to FMM first order phase transition. Our investigations reveal glass–like arrest of kinetics at low temperature which plays a significant role in the thermomagnetic irreversibility observed in this system. Difference in hysteresis thickness with increasing applied magnetic field reveals competition between kinetic arrest temperature and supercooling temperature. Extensive cooling and heating in unequal field (CHUF) measurements are utilized to investigate the glass like arrested states.

j0066

Superconducting properties of 2H-$SnNbSe_2$

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Topological superconductivity, characterized by Majorana zero modes, merges superconductivity with nontrivial topological order. This offers potential for fault-tolerant quantum computation. Transition metal dichalcogenides (TMDs) are promising platforms for exploring these phenomena due to their rich electronic properties, including superconductivity and spin-orbit coupling. This study focuses on polycrystalline 2H-$SnNbSe_2$, which features a unique intercalation of tin (Sn) atoms within $NbSe_2$ layers. We report a superconducting transition temperature T_c of 4.7 K. Magnetization measurements reveal a lower critical field $H_{c1}(0)$ of 24.8 mT and an upper critical field $H_{c2}(0)$ of 1.3 T. These findings highlight the potential of 2H-$SnNbSe_2$ as a possible candidate of topological superconductivity.

j0067

Magneto-transport Properties of Chiral Magnet $Co_8Zn_8Mn_4$: Role of Spin Fluctuations

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The β-Mn type cubic Co-Zn-Mn alloys have recently attracted significant interest for their capability to host skyrmions at room temperature. This study explores the magneto-transport properties of $Co_8Zn_8Mn_4$, emphasizing the role of different scattering mechanisms in the presence of topological invariance. Over a broad temperature range of 55K to 300K, negative magnetoresistance has been observed. In isothermal magnetoresistance curves, a shift from the dominance of magnons to spin fluctuation is suggested by the change in the shape of MR from linearity (for $T << T_c$) to non-linearity (for $T < T_c$ and $T \sim T_c$). The relationship between the anomalous Hall effect and longitudinal resistivity indicates the dominance of the skew-scattering mechanism, challenging the semiclassical magneto-transport theories. We show experimentally that skew scattering in $Co_8Zn_8Mn_4$ originates from the spin fluctuation. As the semi-classical magneto-transport theories cannot explain the dominance of skew scattering in the low conductivity $Co_8Zn_8Mn_4$ compound, our findings shed new light on the role of spin fluctuations, potentially enhancing our understanding on the magneto-transport of low conductivity materials.

j0068

Induction Heating Performance and Cell Viability Analysis of Superparamagnetic $NiFe_2O_4/Fe_3O_4$ Nanocomposites for Hyperthermia Applications

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Tumors are undefined multiplication of cells, which arise from extrinsic sources like physical, chemical, and biological carcinogens. To treat tumors, we synthesized novel $NiFe_2O_4/Fe_3O_4$ nanocomposites (NCs) using the chemical co-precipitation technique. X-ray diffraction (XRD) confirmed the cubic structure with an average size of 12 to 30 nm. The morphology was observed using high-resolution transmission electron microscopy (HR-TEM) and revealed an agglomerated spherical shape with an average particle size of about 20 nm. The incorporation of Fe_3O_4 in $NiFe_2O_4$ (20 and 40 % weight ratios) nanoparticles (NPs) exhibited a higher saturation magnetization (M_s) with superparamagnetic behavior and uniaxial anisotropy. Further, the heating efficiencies were measured using an infrared thermographic camera and an induction heating system with a fixed amplitude and frequency. The maximum specific absorption rate (SAR) of about 414 W/g was observed for the 2NF nanocomposite sample with the required temperature (43 ˚C) for employment in improved hyperthermia therapy. Further, the selectivity index for the prepared nanocomposites in lung adenocarcinoma is 3.3 at 30 μg/ml.

j0069

Characterization of CeO_2 Nanoparticles with Er^{3+} Doping: Insights from X-ray Diffraction to Magnetic Behavior

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This work reports the synthesis and characterization of Er doped CeO_2 nanoparticles prepared by the combustion method. X-ray diffraction patterns revealed that all the synthesized samples dominate CeO_2 cubic fluorite structure. Absorption spectra analyses report a decrease in bandgap energy for Er-substituted CeO_2 samples from 3.013 to 2.81 eV. The ferromagnetic properties of the samples have been investigated at room temperature by the vibrating

sample magnetometer. The origin of magnetism in pure and doped CeO_2 system has been analyzed through F-center mechanism.

j0070

Evidence of Spin-Phonon Coupling in Quasi-Two-Dimensional $La_{1.4}Sr_{1.6}Mn_2O_7$ bi-layer Manganite

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Since the discovery of the presence of magnetic bi-skyrmionic spin texture in layered (n=2) Ruddlesden-Popper series manganite $La_{2-2x}Sr_{1+2x}Mn_2O_7$, there has been a renewed effort to understand the spin-spin interactions in these materials. In this work, we have investigated the tetragonal double-layered $La_{1.4}Sr_{1.6}Mn_2O_7$ (x=0.3). Multiple magnetic and electric phase transitions were found at T_{C1} (~101K), T_{C2} (~246K), and T_{C3} (~295K) in this system. The compound emerged from ferromagnetic metallic (FMM) to paramagnetic insulator (PMI), passing through two types of canted antiferromagnetic (CAFM) phases. We have used temperature-dependent micro-Raman study over the temperature range from 80K to 450K to investigate the lattice dynamics and spin-phonon coupling across different magnetic phases of the system. The anomalous softening of Raman shift across different magnetic phases is attributed to spin-phonon coupling induced by magnetic exchange interaction due to competition between the nearest neighbor (NN)and the next nearest neighbor (NNN) spin-spin interaction in the 2D MnO_2 plane. The relative magnitudes of NN and NNN spin-phonon coupling strength in the FMM and CAFM phases are estimated.

j0071

Resistively capacitively shunted junction model analysis of YBCO step edge junction

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Step edge Josephson junction is fabricated using pulsed laser deposited YBa2Cu3O7-x (YBCO) film on step etched single crystal MgO (100) substrate. A step of height ~ 400 nm and angle ~ 35° is fabricated on MgO substrate using photolithography and ion beam etching (IBE) techniques before the deposition of thin film. After the deposition of YBCO film on the step etched MgO substrate, a microbridge with width of 2 μm and length of 100 μm is fabricated over the step, and its transport properties are studied. The DC Josephson effect of the step edge junctions at 75 K is observed and modelled using the resistively capacitively shunted junction (RCSJ) model using MATLAB. The simulation results suggest that instead of a single junction, the step edge Josephson junction consists of two junctions connected in series. Possibly the top and bottom edge of the step are acting as the two junctions with the top edge acting as weaker one among the two.

j0072

Magnetic Properties and Magnetocaloric Effect of Cr_3Te_4

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The binary layered monoclinic telluride, Cr_3Te_4, is potential topological material and has it ferromagnetic Curie temperature above room temperature. To study the magnetic and thermal properties of this important compound detailed dc magnetization and heat capacity measurements were carried out. Cr_3Te_4 orders ferromagnetically at 323 K and as T is lowered it undergoes FM to AFM like transition around 90 K. The magnetization results indicate that the low temperature phase is not a pure AFM phase but the spin structure seems to have canted structure. And the AFM component arising from this canted of spin structure. This phase is still dominantly FM with AFM component being relatively small. Heat capacity (C_p) shows a peak around T_C but no clear transition around 90 K is seen. Only feeble slope change is noticed indicating change in spin structure is not dramatic. Analysis of C_p data yields the Sommerfeld coefficient, γ = 17.3 mJ/(mol K^2), and the Debye temperature as θ_D ~ 202 K. The MCE analysis shows the maximum values of - ΔS_M and RC values as ~3.2 J/Kg-K and 143.8 J/kg. respectively. The MCE parameters obey universal scaling laws as predicted by mean field theory for second order magnetic transition.

j0074

Exploration of Structural and Magnetic Properties of Nd-doped $LaCrO_3$

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In this paper, we investigate the structural and magnetic properties of polycrystalline $La_{1-x}Nd_xCrO_3$ (x = 0.00, 0.05, 0.15). All the samples were synthesized using the solid-state reaction method. The structural characterization, like phase purity, crystal structure, and surface morphology, was performed through X-ray diffraction (XRD) and field emission scanning electron microscopy (FESEM) techniques. Room-temperature Raman spectroscopy revealed the presence of 11 active modes at 514 nm laser excitation for all the samples. The Neel temperature (T_N) decreases with increasing Nd doping. This indicates that the strength of the Cr^{3+}-Cr^{3+} interaction decreases with Nd substitution. A spin-reorientation transition was observed at low temperatures only for substituted samples. The substitution of Nd introduces an exchange bias within the samples and the maximum exchange bias field (H_{EB}) is found to be -674Oe for x=0.15 sample.

j0077

Impact of Structural Transition on Magnetic and Electrical Behavior in Pr and Co Doped $BiFeO_3$ Nanoparticles

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This study explores the magnetic and electrical properties of Pr and Co co-substituted BiFeO3 (BFO) nanoparticles, emphasizing the effects induced by structural transitions. BiFeO3 is renowned for its multiferroic nature, displaying both ferroelectric and magnetic properties, making it a prime candidate for applications in spintronics and memory devices. By incorporating Pr and Co as co-substituents, this research aims to enhance the intrinsic properties of BFO nanoparticles. Structural characterization through X-ray diffraction (XRD) conducted to analyze phase transitions. Magnetic properties were assessed using a vibrating sample magnetometer (VSM), while dielectric measurements were employed to evaluate electrical properties. The results reveal that Pr and Co co-substitution significantly influences the structural transition, resulting in enhanced magnetic and electrical behavior. The improved ferroelectric and ferromagnetic properties of Pr and Co co-substituted BiFeO3 nanoparticles can be attributed to the synergistic effects of the dopants on the crystal structure and charge distribution. This study offers valuable insights into designing advanced multiferroic materials with tailored properties for next-generation technological applications.

j0080

Structural and Magnetic Properties of Sm_2FeCrO_6

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This study synthesized the double perovskite Sm_2FeCrO_6 (SMFCO) using the conventional sol-gel method. XRD analysis with Rietveld refinement confirmed the orthorhombic structure with space group *Pbnm* (62). The parameters of lattices were found to be a = 5.2629 Å, b = 5.4203 Å, and c = 7.5037 Å, along with a unit volume of 214.055 $Å^3$. FESEM analysis revealed spherical particles with an average grain size of ~ 330 nm, while EDX spectra verified the presence of Sm, Fe, Cr, and O. Magnetic measurements identified a transition temperature at 260 K, associated with G-type canted antiferromagnetic ordering. Below this temperature, hysteresis suggests weak ferromagnetism, whereas above it, the compound exhibits paramagnetic behavior.

j0081

Inhomogeneous melting of vortex lattice in superconducting thin films of MoGe

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Vortex liquid can exist for a large part of phase diagram of thin film superconductors due to higher susceptibility of two-dimensional vortex lattice to thermal and quantum fluctuations. Here we report formation of vortex liquid state at low magnetic field and temperature in superconducting thin films of amorphous MoGe. However, a series of vortex

images taken consecutively by scanning tunneling spectroscopy (STS) reveals that the liquid state is inhomogeneous in nature where we observe both static and moving vortices in a mixed landscape.

j0082

Nematicity and vortex activation in single crystal $FeSe_{0.4}Te_{0.6}$ superconductor

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In this paper, we try to investigate the nematic phase and vortex pinning mechanism in Iron-based superconductor $FeSe_{0.4}Te_{0.6}$. Previous studies show the emergence of nematicity in FeSe around 90K. The presence of nematic phase results in a kink or change in slope in resistivity because of the anisotropy in the electronic structure which occurs due to phase transition from tetragonal to orthorhombic. $FeSe_{0.4}Te_{0.6}$ single crystals were prepared through self-flux method. Structural analysis was carried out by XRD measurement which confirms the formation of tetragonal phase structure of $FeSe_{0.4}Te_{0.6}$ single crystal. Resistivity vs temperature shows T_c of 14.2K. But no anomaly in resistivity is observed in our sample. This means that substitution of Te around $x\approx0.6$ suppresses the nematic phase. We got clear evidence for the presence of superconductivity with $T_c\approx14.2$ K supported by resistivity, and magnetization measurements. The vortex activation energy is also estimated from the Arrhenius

j0083

Low Frequency Electrodynamics of A Pinned Vortex Liquid

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In a 5 nm thin film of amorphous Re_6Zr (a-ReZr), the vortex lattice, typically observed in superconductors, behaves differently due to its susceptibility to thermal fluctuations. Unlike conventional superconductors where the vortex lattice solidifies, the vortex liquid state in a-ReZr persists down to low temperatures and fields without transitioning into a glassy or solid state. This study investigates the compressibility of the vortex liquid under various conditions. Using a mutual inductance setup, an AC current generates oscillatory supercurrents in the film, causing vortices to oscillate and induce voltage in a secondary coil. This setup measures the compressibility of the vortex system by observing the in-phase and out-of-phase components of the induced voltage. Experimental results show that at higher frequencies, the pinned vortex liquid exhibits shear thickening, similar to non-Newtonian fluids. As frequency increases, vortices have less time to respond, requiring higher magnetic fields to transition into an isotropic liquid state. At 2 K, a clear frequency dependence is observed, while at 0.41 K, the frequency dependence is less pronounced. These findings suggest that the pinned vortex liquid in a-ReZr behaves similarly to a compressible, non-Newtonian fluid.

j0084

Study of optical conductivity in the parent compounds of cuprates across the Mott-insulating phase

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We explore the correlation between the insulating phase and AFM order, the nature of conductivity in the crossover of the insulating to the metallic phase, and the effect of on-site coulomb repulsion on charge localization and conductivity across the Néel temperature. For this, we adopt one-orbital Hubbard model in a square lattice including nearest-neighbor hopping t and onsite coulomb repulsion U, and simulate the system via the Monte-Carlo method by cooling down the temperature in small steps. Our findings underscore the influence of U on metal-insulator transition (MIT) and Néel temperature (T_N), the existence of the paramagnetic insulator above T_N. Above MIT temperature, we also observe a non-Drude like conductivity curve and the existence of a peak at a finite value of ω, indicating the existence of a pseudogap (PG) like features. We also notice shifting of a peak away from $\omega = 0$ with increasing U, indicating the enlargement of the PG phase.

k) ENERGY MATERIALS

k0002

Synthesis and Structural Study of Pre-lithiated Silicon Anode in Different Atmospheric Conditions

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Li-ion batteries are regarded as the groundbreaking development in the field of energy storage. Advanced synthesis of material with increased energy density and cycle stability are of significant priorities in meeting the particular and growing demand for energy storage devices. Si is regarded as a good anode material since it has the highest lithiated phase. Its theoretical capacity is around 4199 $mAhg^{-1}$, which is about ten times that of graphite used in conventional batteries. In practical applications, excessive volume expansion during silicon lithiation can lead to lithium loss within the battery unit, reducing its capacity and causing electrode failure or cracking. To address this issue, a pre-lithation procedure was proposed. In this study, a pre-lithiated sample of the most lithiated Li-Si ($Li_{21}Si_5$) phase of Li-Si alloy is primed using the melt solidification method in different atmospheric conditions and structural study is reported and observed.

k0003

Supremacy of Dual Absorber Layer Based QDSC over Single Absorber Layer Based QDSC

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Quantum dot solar cells, utilizing single absorber layers, have been explored over the past few decades, yet have only achieved laboratory efficiencies less than 20%. To enhance the efficiency of these solar cells by improving the absorption of incident solar energy photons, the concept of a dual absorber layer was introduced. For this purpose, two commonly used quantum dot absorber materials, PbS QD and CZTS-QD, have been employed. The difference in their bandgaps allows for varied photon absorption, enabling a broader portion of the solar spectrum to be converted into electrical energy, thus enhancing the performance of the dual absorber layer quantum dot solar cell. An impressive efficiency of 27.85% has been attained with the PbS-CZTS dual absorber layer QDSC.

k0004

Exploring $ZnFe_2O_4$ Hollow Microspheres as Supercapacitor Electrode Material

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Herein, we have reported the structural, microstructural and electrochemical properties of $ZnFe_2O_4$ hollow microspheres synthesized by solvothermal technique. The sample has been characterized by recording the powder x-ray diffraction (PXRD) pattern, electron microscopic images using field emission scanning electron microscopic (FESEM) and high-resolution transmission electron microscopic (HRTEM) techniques. The sample is cubic spinel having $Fd\bar{3}m$ space group and composed of hollow microspheres with average diameter of 326.4 nm and shell thickness of 58 nm. According to N_2 adsorption-desorption study, the pore size and BET surface area are 2.77 nm and 24.54 $m^2\ g^{-1}$, respectively. The sample exhibits pseudo capacitive behavior with an impressive high specific capacitance value of 993.8 F g^{-1} at 5 mV s^{-1}. Interestingly, the value of the specific capacitance of the sample is found to be increased by 34% after 1000 cycles of galvanostatic charging-discharging.

k0005

Effects of different mass loading of La_2NiCrO_6 on the electrodes in supercapacitor performance

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With the growing demand for portable devices, developing high-performance electrodes for energy storage systems has become a substantial challenge. The critical point for fabricating high-performance equipment is choosing the appropriate electrode materials with optimized electrode parameters. This work proposes lanthanum-based double perovskite material La_2NiCrO_6 (LNC) as a potential electrode material for supercapacitor positive electrode. The proposed LNC material is synthesized using sol-gel followed by a solid-state reaction route. Material confirmation and morphological studies are done using XRD and SEM analysis. A series of electrochemical studies such as galvanostatic charge-discharge (GCD), cyclic voltammetry (CV), and impedance spectroscopy (EIS) are done on the

electrodes coated with different mass loading from 0.4 mg to 8 mg (0.4, 0.8, 2, 4, and 8 mg) of active materials. The electrode coated with 0.4 mg of active material exhibits the highest specific capacity of 406 C g^{-1} at the specific current of 1 A g^{-1}, and it displays 90% capacity retention and 99% Coulombic efficiency at the specific current of 10 A g^{-1}.

k0006

Impact of Electrolytic Cations in the Pseudocapacitive Performance of $SrFeO_{3-\delta}$

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This work investigates the effect of cations in the electrolyte on the pseudocapacitive performance of $SrFeO_{3-\delta}$. $SrFeO_{3-\delta}$ is synthesized using the sol-gel method, and its structure is analyzed by XRD. Electrochemical studies are conducted in 2 M LiOH, 2 M NaOH, and 2 M KOH using a three-electrode system. $SrFeO_{3-\delta}$ exhibits the highest specific capacity of 338.6 C/g at 1 A/g and retaining 50% of its capacity after 6000 cycles.

k0007

Mechanical and Electronic Properties of Double Perovskite K_2TlInF_6: A DFT study

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The structural, mechanical and electronic properties of double perovskite K_2TlInF_6 are investigated in the current work using the Density Functional Theory in combination with the full potential Linear Augmented Plane Wave (FP-LAPW) method. PBE-GGA potential is used to approximate exchange correlation potential. The structural parameters and elastic constants analysis shows the studied compounds are stable and ductile.The Band Structure reveals the p-type semiconductor nature of the material with an indirect band gap. TDOS further confirms the results obtained from energy band plots.

k0008

Rod-shaped nanostructured Mn-doped CuO Electrocatalyst for oxygen evolution reaction

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This study explores synthesizing and characterizing Mn-doped CuO to optimize its electrocatalytic performance for oxygen evolution reaction in water splitting. A novel rod-shaped nanostructured Mn-doped CuO was prepared using the solvothermal synthesis methodology. Electrochemical evaluations in 1.0 M KOH showed the fabricated rod-shaped nanostructured CuO doped with 0.23 at % Mn catalyst achieves a current density of 10 mA cm^{-2} at an overpotential of 319 mV vs. RHE, with a Tafel slope of 120 mV dec^{-1}.

k0010

Anharmonic atomic dynamics and thermal transport in SnTe

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We have comprehensively investigated the anharmonic lattice dynamics in SnTe and Sn0.9Te. We identified the presence of fourth-order anharmonicity, which leads to suppressed lattice thermal conductivity in SnTe. The presence of Sn vacancies further enhances the acoustic phonon scattering and further reduces the lattice thermal conductivity.

k0011

Effect of Addition of Pb_3O_4 on the energy Release of Al/CuO Nanothermite

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The synthesis of Al/CuO/Pb_3O_4 nanothermites is accomplished using the physical mixing approach with the assistance of ultrasonication. Pb_3O_4 is included as a secondary oxide in these nanothermites. X-ray diffraction was performed on these nanothermites to analyze the crystalline phase of their components. The thermite reaction of Al/CuO/Pb_3O_4 nanothermites with varying compositions was investigated using differential scanning calorimetry. The study revealed that the energy release of Al/CuO nanothermite was enhanced on the addition of Pb_3O_4.

k0013

Examining Potential Of $Mn_{0.7}Zn_{0.3}Fe_2O_4$ Solid Microspheres As Supercapacitor Electrode Material: Study On Its Electrochemical Performance

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The structural, microstructural characteristics and electrochemical supercapacitive behavior of $Mn_{0.7}Zn_{0.3}Fe_2O_4$ solid microspheres synthesized by template-free solvothermal method have been reported here. The powder x-ray diffraction (PXRD) and Fourier transform infrared (FTIR) spectroscopic studies confirm that the sample is well crystalline (~ 43.25 nm), single phase cubic spinel ferrite of $Fd\bar{3}m$ symmetry. The field emission scanning electron microscopic (FESEM) and transmission electron microscopic (TEM) techniques confirm that the individual microspheres having average diameter ~ 248 nm are composed of constituent nanoparticles of size ranging between 10 – 14 nm. The sample exhibits excellent electrochemical behavior with specific capacitance of 2193 F g^{-1} at 2 mV s^{-1} and has long life cycle with 94 % capacitance retention over 1000 cycles. Thus, the sample is promising electrode material for supercapacitor application.

k0014

Relaxor SBT/PVDF-HFP Ferroelectric Flexible Films for Energy Storage and Harvesting Application

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The eco-friendly $Sr_{0.7}Bi_{0.2}TiO_3$ (SBT) via solid-state sintering method was synthesized. The SBT composition was combined with PVDF-HFP polymer via solution casting to fabricate flexible particulate composites. Characteristic peaks of PVDF-HFP polymer with reflections corresponding to the SBT phase were observed from XRD patterns. SEM micrograph shows homogeneous and spherulite structures which are clearly distinct in the composite film. Enhanced breakdown strength (E_b) of 700 kV/cm was found in 30 wt% SBT/PVDF-HFP. W_{rec} of 64 mJ/cm^3 was estimated which strengthened its potential in energy storage applications. Moreover, Piezoelectric Energy harvester (PEH) fabricated using SBT ceramic-infused PVDF-HFP films shows a voltage output of 6V and~ 13V through different external forces.

k0015

Studies on Ionic Diffusion in $La_{0.57}$ $Li_{0.29}TiO_3$ using Molecular Dynamics Simulation

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Perovskite structured lanthanum lithium titanium oxide i.e. $La_{(2/3-x)}$ $Li_{3x}TiO_3$ ($0.04 < x < 0.16$) shows very high lithium ion conductivity, well known as one of the potential candidates for solid electrolyte. In this work we have extensively studied the lithium ion diffusion in $La_{0.57}Li_{0.29}TiO_3$ at different temperature using large scale molecular dynamics simulations. We found that, at 800K lithium ion show two-dimensional diffusion along the ab-plane with diffusion constant about 6.77×10^{-6} cm^2/sec and activation energy ~0.33 eV, which is in fair agreement with reported values. We have shown that vacancy playing an important role for lithium-ion diffusion in $La_{(2/3-x)}$ $Li_{3x}TiO_3$ ($0.04 < x < 0.16$) and lithium ion diffuse through vacancy hopping mechanism within the bottleneck of TiO_6 octahedra.

k0016

Synthesis of Fe doped $MnCo_2O_4$ Nanoparticles for Supercapacitor Application

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In this study, we have synthesized $MnCo_2O_4$ nanoparticles doped with Fe (0.2, 0.4, and 0.6) using a hydrothermal method. The crystal structure and morphology of the fabricated materials were analyzed using X-ray diffraction and field-emission scanning electron microscopy (FE-SEM). Fourier-transform infrared spectroscopy (FTIR) was used to analyze the presence of functional groups. The electrochemical properties of the prepared samples were studied using an electrochemical workstation with a two-electrode setup in a 3 M KOH electrolyte.

k0018

Prussian Blue as Cathode Material for Ultra Stable Aqueous Ammonium Ion Batteries

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The Prussian blue (PB) and its analogues (PBAs) are extensible studied for Li, Na, and K ion batteries; however, lower specific capacity and poor cyclic stability makes them undesirable for commercial applications. Herein, we demonstrate that PB material is highly suitable for ammonium ion (NH_4^+) batteries with improved cyclic stability. Thin film of PB is electrochemically synthesized on glossy carbon electrode and characterised using cyclic voltammetry (CV) and galvanostatic charging-discharging (GCD) for cathode material of aqueous ammonium ion batteries. The CV shows that PB film found to be electrochemical active and exhibit a pair of redox peaks due to Fe^{+2}/Fe^{+3} metal ions. For ammonium ion insertion and extraction, 0.1 M $(NH_4)_2SO_4$ electrolyte is used which exhibit three redox peaks, manifested due to ammonium ions. The GCD study reveal that the material is very stable and does not degrade at higher current density and number of cycles. The specific capacity and specific capacitance are found to ~1.5 µAh/cm^2 and ~12 mF/cm^2 respectively at current density of 10 µA. The values of specific capacitance and specific capacity remain constant even after 60 cycles confirm that the material is ultra-stable for aqueous ammonium ion batteries.

k0019

Inelastic Neutron Scattering and ab-initio molecular simulations of Li_xMPO_4 (x =0,0.75,0.5; M = Fe, Mn)

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Lithium transition metal phosphor-olivines are useful electrode materials, owing to their stability, high safety, low cost and cyclability. Despite enormous works pertaining to battery research, many aspects of their basic vibrational and other physical properties have not been completely understood. Here we report the inelastic neutron scattering studies of the vibrational behavior of these compounds compared to our computed ab-initio molecular dynamics simulations. We have tried to understand the effect of delithiation on diffusivity of Li atoms, which are crucial in their applications as cathode materials.

k0021

Study of Nickel Cobalt Oxide as an Electrocatalyst for Oxygen Evolution Reaction in Wide Range of Alkaline pH

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The present study was undertaken to determine the electrocatalytic performance of solvothermally synthesized nickel cobalt oxide for Oxygen Evolution Reaction (OER) in water splitting at different pH. The synthesized electrocatalyst shows spherical flower-like morphology. OER activity increased with increasing pH (pH 8.2 < pH 10.4 < pH 12). The electrocatalyst performs best in extreme alkaline pH. For pH 12, an overpotential of 346 mV vs. RHE at 10 mA cm^{-2}, a Tafel slope of 167 mV dec$^{-1,}$ and an exchange current density of 0.041 mA cm^{-2} are observed.

k0022

Antimony Sulfide Composite as High-Performance Anode Material for Lithium-Ion Battery

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One of the alternatives to the existing low performing graphite anode material is antimony sulfide (Sb_2S_3). This is due to its favorable layered structure, fairly good electrical conductivity and high theoretical capacity. However, due to large volume changes during charge-discharge reactions, the cycle stability and the rate performance are not satisfactory. To overcome this issue, Antimony sulfide composite with PANI (polyaniline) was synthesized. Sb_2S_3 was synthesised by hydrothermal method followed by wet chemical synthesis for Sb_2S_3 composite with PANI and this procedure was optimised to obtain single phase antimony sulfide. All the XRD diffraction peaks were indexed to the orthorhombic phase of Sb_2S_3, space group Pbnm (ICSD collection code 26751). FTIR spectrum of Sb_2S_3 shows the band corresponding to symmetric and asymmetric vibrational mode of Sb-S-Sb at 561 and 700 cm^{-1} respectively while Sb_2S_3-PANI shows the bands at 800, 1100, 1400 cm^{-1} and 2900-3300 cm^{-1} supporting the presence of PANI in the composite. The Sb_2S_3 – PANI shows the initial discharge capacity of around 878 mAhg-1 and initial coulombic efficiency of 82.9%. It gave a reversible specific capacity of 590 mAhg-1 for 100 cycles at a current rate of 50mAg^{-1}. The cyclic voltammetry confirmed the reversible nature of charge-discharge reaction and the alloying and conversion reaction of Sb_2S_3 with Li^+. The remarkable increase in performance of Sb_2S_3 – PANI is due to the cushioning effect of PANI matrix which accommodates the volume change and reduces the pulverization of electrode during operation of cell. PANI also enhances the electrical conductivity and increases Li^+ diffusion rate. High current rate and rate capability tests also endorsed the enhanced performance of Sb_2S_3 – PANI composite.

k0023

Graphite Sintered Strontium Praseodymium Titanate Perovskite For Thermoelectric Applications

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Pr^{3+} was introduced in the Sr^{2+} site in $Sr_{1-x}Pr_xTiO_3$ (x=0.05, 0.075, 0.10, 0.125, 0.15, 0.20) system followed by two step graphite burial sintering. Powder reduction helps to increase the carrier concentration and the doped sample pellet reduction minimizes Double Schottky Barrier generated by strontium and oxygen vacancies at grain boundary by regulating the point defects. Samples with $x \geq 0.10$ shows splitting and asymmetry of (200) and (310) peak in XRD indicating structural transformation from cubic to tetragonal phase. XPS spectra of the samples confirmed the formation of oxygen vacancies and reduction of Ti^{4+} to Ti^{3+} induced by graphite burial sintering resulting in enhanced carrier concentration. A maximum power factor of 1.8 mW/mK^2 was obtained for $Sr_{0.9}Pr_{0.1}TiO_3$ samples at 673 K. Reduced thermal conductivity due to porous structure, Pr defect centers, oxygen vacancy clusters together with enhanced power factor lead to a maximum figure of merit 0.33, making this an ideal candidate as n type legs in thermoelectric generators.

k0025

$Li_7La_3Zr_2O_{12}$: A Solid State Electrolyte Towards Thin Film Battery

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The growth of $Li_7La_3Zr_2O_{12}$ (LLZO) thin films on glass substrates using radio frequency (RF) sputtering at 50W of RF power is investigated. As-deposited films were annealed at 500ºC. Results from Rutherford Backscattering Spectrometry (RBS) indicate that La, Zr and O are present in as-deposited and annealed films. The thicknesses of both films are 100 nm approximately. The thickness of annealed film estimated from scanning electron microscopic (SEM)

measurement is 46 nm. The amorphous character of the film is revealed by X-ray Diffraction (XRD) measurement. Near edge X-ray absorption fine structure (NEXAFS) reflects structure corresponding to the interaction between oxygen ions and metal ions locally.

k0026

Synthesis and Cyclic Voltammetric Studies of Co doped $NiFe_2O_4$ Nanoparticles for Energy Storage Applications.

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This work focuses on the synthesis and electrochemical properties of cobalt-doped nickel ferrite ($NiFe_2O_4$) with varying cobalt concentrations (0, 0.1, 0.2, and 0.3 mol%). Both pure nickel-ferrite and cobalt-doped nickel-ferrite nanoparticles were synthesized using the hydrothermal technique. X-ray diffraction (XRD) was used to investigate the crystallinity of the produced samples. Using cyclic voltammetry (CV) study analysis and 3 M KOH electrolyte solution, the electrochemical behavior of the produced samples was examined. With different scan rates of 1, 2, 3, 4, and 5 mV/s, the potential window was restricted to 0 V to 0.4 V. According to a cyclic voltammetry investigation, the specific capacitance was raised higher by the cobalt dopant than by pure nickel ferrite. Among the samples, the one with 1 mol% cobalt doping exhibits the highest specific capacitance, indicating optimal electrochemical performance. These findings underscore the potential of cobalt-doped nickel ferrite as a high-performance material for energy storage applications.

k0027

$SrMnO_3$ Perovskite Nanoparticle Embedded in $NiCo_2O_4$ Nanoflower as Electrocatalyst for Oxygen Evolution

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Designing high-efficiency, stable, and inexpensive electrocatalysts for oxygen evolution reaction (OER) is essential. In this work, we have synthesized a composite of perovskite $SrMnO_3$ and spinel $NiCo_2O_4$ by a hydrothermal process. The obtained $SrMnO_3/NiCo_2O_4$ exhibits an overpotential 489 mV at current density 10 mA/cm^2 and Tafel slop 97 mV/dec in alkaline media and electrochemical surface area 2.88 cm^2 as calculated from CV.

k0028

Two-Dimensional Be_2P_4/BP Heterostructure as an Anode Material for Sodium-Ion Batteries

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To explore the electronic and electrochemical properties of two-dimensional (2D) Be_2P_4/BP heterostructure, density functional theory (DFT) has been employed. The electronical properties of monolayer Be_2P_4 and BP indicate their semiconducting nature having band gaps of 0.5 eV and 0.89 eV, respectively. In addition, we also studied adsorption and storage phenomenon of van der Waals Heterostructure (vdWH) combining Be_2P_4 and experimentally synthesized BP monolayer. The calculated electronic band structure of Be_2P_4/BP heterostructure clearly illustrates semiconducting nature with bandgap of 0.16 eV which changes into metallic during the adsorption of Na atom with high adsorption energy. The computed high specific capacity and low OCV make Be_2P_4/BP heterostructure an appealing choice for energy storage applications.

k0029

Few Layered $Mo_3C_2T_x$ Based MXene Electrodes for Efficient and Stable Symmetric Supercapacitor

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In the present work, a novel two-dimensional few layered $Mo_3C_2T_x$ MXene was employed as an active electrode material for developing efficient symmetric supercapacitor (SSC); exhibited improved electrochemical performance than other transition metal based MXenes due to their remarkable optoelectronic and electrochemical properties,

tunable physiochemical properties and possesses high thermodynamic and chemical stability. The few layered **$Mo_3C_2T_x$ - based SSCs outcase the enhanced electrochemical performance** exhibited maximum specific capacitance of 150.48 Fg^{-1} at current density of 0.2 Ag^{-1}, capable of delivering a high energy density of **83.6 Wh kg^{-1} over longer duration of period which was confirmed through** cyclic voltammetry and galvanostatic charge-discharge.

k0030

Electrochemical Synthesis Of Nickel Hydroxide, Cobalt Hydroxide And Their Layered Double Hydroxide For Supercapacitor Application

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In the present investigation, Nickel hydroxide ($Ni(OH)_2$), Cobalt hydroxide ($Co(OH)_2$) and ($Ni(OH)_2/Co(OH)_2$) layered hydroxide (LDH) thin films were deposited on stainless steel (SS) substrate potentiostatically. Thin film deposition parameters like concentration of solution and time for deposition were optimized. These thin films were characterized using Raman spectroscopic technique. Electrochemical characterizations i.e. Cyclic Voltammetry and Galvanostatic Charge Discharge of these films were studied for supercapacitor application.

k0031

Hydrothermal Synthesis of α-MnO_2 and β-MnO_2 Nanorods as Cathode Materials for Aqueous Zinc Ion Batteries

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In the recent years, world has seen a tremendous increase in the usage of energy. The advancement in technology, artificial intelligence are some reasons for these. In this study α-MnO_2 and β-MnO_2 is synthesized through hydrothermal method to study and compare the electrochemical performance of these materials as cathode in aqueous Zinc ion Batteries (ZIBs). Further to confirm the proper phase formation it is characterized by XRD, FTIR and Raman.

k0032

Exploring Supercapacitive property of MoS2/g-C3N4 composites on Screen-printed Carbon Electrode

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One of the most promising energy storage technologies for future generations is the supercapacitor. In this work, 2D MoS2 nanosheets are decorated with 2D g-C3N4 by cost-effective and eco-friendly method. The structure confirmation was done from XRD. The electrochemical characterization techniques such as cyclic voltammetry (CV) from potential range -1 to 1 V, and electrochemical impedance spectroscopy (EIS) 1 Hz to 50 kHz were used to explore the supercapacitive properties of MoS2/g-C3N4 composites on screen-printed carbon electrode (SPCE). The areal capacitance calculated is 6.712 F/cm2 at 10 mV/s in the potential region -1.0 V to 1.0 V. The result manifests that MoS2/g-C3N4 composites can be promising electrode materials for Supercapacitor applications**.**

k0033

Study on Effect of Synthesis Route on the Properties of $LiFePO_4$ for Energy Storage Applications

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The proposed article emphasizes on the synthesis, structural morphological and electrical properties of $LiFePO_4$. The material is coated with carbon materials to improve the electrochemical performance. $LiFePO_4$ nanoparticles is synthesized by solvothermal, sol-gel and solid-state reaction techniques. The phase formation of the material and the

purity of phase of the material synthesized under various synthesizing techniques are studied and confirmed by the X-Ray Diffraction. The chemical bonds of the prepared material are analyzed using FTIR studies. The morphology and grain size of the material is analyzed from FESEM images. The effect of the synthesis route on the size of the particle is studied.

k0034

Inter lamellar porosity by Kirkendall effect and enhanced thermoelectric performancein $CuCrO_2$ crystallites via multi-cation doping (Zn^{2+}, Ni^{2+}, and Mg^{2+})

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Introducing interlamellar porosity is of significant importance as it effectively influences the modulation of both the Seebeck coefficient and thermal conductivity. The layered structure and interlamellarpores emerge as a result of the diffusion of doping cations (Zn^{2+}, Ni^{2+}, and Mg^{2+}), which leads to therepositioning of Cr^{3+} in $CuCrO_2$ crystallites. The intricate structural evolution mechanism is elucidatedthrough the Kirkendall effect and the presence of nanopores, as depicted in FESEM images, with sizes around 100 nm, hinders the movement of phonons, resulting in a minimal conductivity of 2.6 W/mKat 973 K.The achieved electrical conductivity of 4796 S/m at 973 K and the filtering effect of nanopores, along with spin alteration and resulting spin entropy, induced higher Seebeck coefficients of 400 μW/mK at 973 K. The highest power factor obtained here is 588 $\mu W/mK^2$, and the maximum achieved ZT, obtained by optimizing all thermoelectric parameters, is 0.22 at 973 K. We have successfully addressed the primary challenge of the interdependency between various thermoelectric factors and improved efficiency, achieving the highest value among Cu-based delafossites.

k0035

Modulating Perovskite Stability Through Incorporation of 2D Spacer Cations for Solar Cell Application

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Perovskites, despite having excellent opto-electronic properties and low-cost synthesis method, they are still not suitable choice for commercialization because of their instability in ambient environment. A promising strategy to improve stability of perovskite involves the formation of 2D/3D hybrid perovskites by introducing spacer cations into the 3D structure. This study investigates the effect of octylammonium (OA) as a spacer cation in $MAPbI_3$. OA (Octylammonium) incorporation targets defect passivation, aiming to mitigate defects on the surface and grain boundaries of $MAPbI_3$. X-ray diffraction (XRD) and Scanning Electron Microscopy (SEM) were employed to analyse the impact of OA on structural stability and film morphology. The results show that OA (Octylammonium) hinders the ion migration resulting in improved structural stability, potentially leading to more durable and efficient Perovskite Solar cell.

k0036

Bifunctional $NiSe_2$ Nanoclusters for Supercapacitor and Photocatalytic Dye Degradation Applications

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Herein, $NiSe_2$ nanoclusters are synthesized via a hydrothermal route. The structural and morphological analyses confirm the formation of nanoclusters of $NiSe_2$ materials. Electrochemical testing of the $NiSe_2$ for a supercapacitor cell shows a specific capacitance (C_{sp}) of 250 F/g at 10 mV/s. It displays a power density (Pd) of 800 W/Kg and an energy density (Ed) of 21.7 Wh/Kg. The degradation of methyl orange (MO) is used to test the catalytic activity of $NiSe_2$. The $NiSe_2$ exhibits remarkable catalytic performance with a 92% degradation efficiency for MO after 80 minutes in the sunlight. $NiSe_2$ nanoclusters have potential applications in photocatalytic dye degradation and high-performance energy storage.

k0038

Synthesis and Study of Eu^{3+} Doped $NaSrBiTeO_6$ Double Perovskite Red Phosphor

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Efficient red emitting phosphor is crucial for high-quality phosphor-converted white LEDs (pc-WLEDs). Double perovskites doped with Eu^{3+} are widely investigated because of their excellent thermal and chemical stability. In the present work, Eu^{3+} doped $NaSrBiTeO_6$ was prepared by conventional high temperature solid state reaction method by varying the dopant concentration. Structure of the prepared compound was confirmed by XRD study. Optimum dopant concentration was obtained by optical studies confirming its potential as an efficient red phosphor. Morphological observation was also performed on the prepared compound.

k0039

Investigation on Defect Density and Performance of Highly Efficient Photo-Voltaic Formamidinium Tin Iodide Perovskite Solar Cells for Indoor Applications

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Indoor photovoltaic materials with tailored properties to efficiently convert low-intensity light into electricity have significant potential in current time. The remarkable optoelectronic characteristics and lower toxicity of organic-inorganic halide perovskites particularly formamidinium tin iodide ($FASnI_3$) have made them attractive alternatives to lead-based perovskites. This study examines the influence of defects on the performance of $FASnI_3$-based perovskite solar cells under indoor conditions (LED-warm, LED-cool) using SCAPS 1D simulations. We consider the effects of different defect densities (from 10^{13} to 10^{18} cm^{-3}) and types (neutral, donor, and acceptor) in the absorber layer. Our results show that the power conversion efficiency (PCE) of $FASnI_3$ perovskite solar cell is highly dependent on defect type and density with a remarkable efficiency of around 41% under LED-warm indoor conditions.

k0041

Synthesis and Characterization of Lithium and Sodium Nickel Oxides for Application as Cathode Materials

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Sodium nickel oxide and lithium nickel oxide samples were prepared by solid state sintering method in the temperature range: 700-800°C. The materials were characterized by X-ray diffraction and Fourier Transform Infrared Spectroscopy. The electrical conductivity of the materials was carried out by four probe and two probe methods. The X-ray diffraction studies confirmed the formation of crystalline phases. FTIR studies show the stretching vibrations of Ni-O linkages at 700-800 cm^{-1} while the infrared absorption bands in the range of 440-670 cm^{-1} are due to the bending vibration of Ni-O bonds. Both lithium nickelate and sodium nickelate samples show the semiconducting behavior with electrical conductivity of 13.0 $S{\cdot}m^{-1}$ and 4.2 $mS{\cdot}m^{-1}$ respectively.

k0042

Pathway for Enhanced Oxygen Ionic Conductivity in $Cu_2P_2O_7$

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Abstract. Solid oxide fuel cell (SOFC) is characterized by high efficiency, long-lasting, silent operation and affordable technology for producing electricity. Generally, SOFC operates at higher temperature (≥ 1273 K) and significant research efforts are given to lower the working temperature to reduce the operating cost. For this, low activation energy, subsequently, high ionic conductivity of electrolyte at lower temperature is desirable. The present study focuses on the enhancement in ionic conductivity of solid electrolyte $Cu_2P_2O_7$ through vanadium (V) substitution. Oxygen ionic conductivity of $Cu_2P_{1.6}V_{0.4}O_7$ has been investigated by impedance spectroscopy. A reduction in activation energy from 1.47 eV for $Cu_2P_2O_7$ to 1.19 eV for the compound $Cu_2P_{1.6}V_{0.4}O_7$, leading to a 3/2 times enhancement in oxygen ionic conductivity, has been achieved. The conduction mechanism of ionic transport has been determined over the temperature range of 423-993 K, where a correlated barrier hopping (CBH) process

contributes in the low (423-523 K) and high (703-993 K) temperature ranges. A deviation from the CBH process is observed in the intermediate temperature range over 523-703 K, just above the crystal structural phase transition temperature of 500 K.

k0044

Co-precipitation Synthesis of Cobalt Ferrite ($CoFe_2O_4$) Nanoparticles and Their Supercapacitor Applications

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In the present work, we have synthesized the nanocrystalline cobalt ferrite ($CoFe_2O_4$) through co-precipitation method. Investigations carried out using x-ray diffraction, infrared spectroscopy and Raman spectroscopy techniques confirm the purity and single phase formation of spinel $CoFe_2O_4$ (CFO) with $Fd\bar{3}m$ space group. Prepared sample is also tested for its energy storage properties by depositing it on nickel foam and using it as cathode material in a three-electrode setup. The impressive values of specific capacitance achieved for this sample indicates that the material under study is a suitable choice for being used in fabrication of supercapacitors.

k0047

Functionalisation of Selenium monolayer with Platinum dichalcogenide for the green Hydrogen production

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Here, we introduce the design of highly efficient photocatalyst PtS2-Se for the water-splitting hydrogen production by first principle methods. The thermal stability of the designed heterostructure at ambient conditions is studied using ab initio molecular dynamics simulations (AIMD). The electronic band structure of the designed structure shows the visible light active bandgap with high band dispersion. The charge density difference and the band alignment indicate the electron transfer from the conduction band minima (CBM) of Se to the PtS_2 monolayer (ML). At the same time holes transfer from the valance band maxima (VBM) of PtS_2 to Se monolayer. After the heterostructure construction, the band alignment found type II, which is suitable for ideal photocatalyst. The charge distribution, electronic properties and the obtained band alignment show that the designed heterostructure has promising water-splitting capacity.

k0048

Enhanced Photo catalytic Performance of MoS2/bg-C3N4 Hetero-structures for Hydrogen Evolution Reaction: A First-Principles Study

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Abstract: This study investigates the potential of a MoS2/bg-C3N4 heterostructure as a promising photocatalyst for hydrogen evolution. Density functional theory calculations were employed to explore the electronic and structural properties of the composite material. The results indicate a significant modification of the electronic structure, with a reduced bandgap and enhanced charge separation due to the formation of the heterojunction. The optimized electronic properties facilitate electron transfer, thereby improving the efficiency of hydrogen production. These findings suggest that the MoS2/bg-C3N4 heterostructure is a promising candidate for developing efficient photocatalysts for sustainable energy conversion.

k0049

Design of high efficiency inorganic perovskite solar cells by numerical simulations

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Inorganic perovskite solar cells (IPSCs) have drawn great research attention because of their outstanding chemical and thermal stability. However, the conversion efficiency of IPSCs is affected from carrier recombination arising due to unfavorable energy level alignment. Therefore, selection of suitable electron transport layer (ETL) and hole transport layer (HTL) is very crucial for the design of high efficiency IPSCs. Here, we propose *n*-MgZnO and *p*-CuO layers as ETL and HTL for inorganic perovskite $CsSnX_3$ (X=I and Br) solar cells, which provides favorable band alignment with absorber layer for seamless electron and hole transport. The numerical simulation data reveals that the $CsSnBr_3$ cell deliver high efficiency of 15.5 % for 800 nm absorber layer thickness, while $CsSnI_3$ has maximum efficiency of 13.4% at lower absorber layer thickness of 300 nm. This work provides great insight for the experimental design and development of high efficiency IPSCs with *n*-MgZnO (ETL) and *p*-CuO (HTL) materials.

k0050

Cyclo[2n]Carbons through the Lens of Density Functional Theory: Role of Rh-decoration in Hydrogen Evolution Reaction

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This study investigates the HER activity of cyclo[6]carbon, cyclo[8]carbon, cyclo[10]carbon, cyclo[12]carbon, cyclo[14]carbon, and cyclo[18]carbon. The cyclo[10]carbon, cyclo[14]carbon, and cyclo[18]carbon have already been synthesized while cyclo[6]carbon and cyclo[12]carbon are claimed to be successfully synthesized. Negative formation energy and all the positive frequencies in the IR spectrum confirm the possibility of natural existence for cyclo[8]carbon. Pristine cyclo-carbon structures are ineffective for HER, exhibiting Gibbs free energy values significantly distant from zero. To enhance their catalytic performance, we decorated each cyclo-carbon ring with rhodium (Rh) atom. The highly negative binding energies indicate a strong interaction between the Rh atom and the cyclo-carbon ring. The Gibbs free energy changes (ΔG_H) for the Rh-Functionalized structures were -0.12 eV, 1.35 eV, -0.13 eV, 0.03 eV, 2.24 eV, and -0.04 eV, respectively for cyclo[6]carbon, cyclo[8]carbon, cyclo[10]carbon, cyclo[12]carbon, cyclo[14]carbon, and cyclo[18]carbon. These results suggest that Rh-Functionalized cyclo[8]carbon and cyclo[14]carbon are unsuitable for HER, while Rh-decorated cyclo[12]carbon and cyclo[18]carbon demonstrate the highest catalytic activity among the studied catalysts.

k0052

Manganese Cobaltite Based Ternary Composite as Efficient Electrode Material for Hybrid Supercapacitors

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The development of proficient electrode materials is one of the major tasks faced by modern techniques for energy storage. Integrating different materials with synergistic effects can be a valuable strategy for designing storage devices with high capacity and energy density. Herein, the $MnCo_2O_4$/AC/PPY ternary composite has been synthesized by a facile approach. The optimized ternary composite (MAP-20) exhibited a capacitance of 945.77 F g^{-1} at five mV s^{-1} compared to pristine $MnCo_2O_4$ (254.98 F g^{-1}). The asymmetric device with MAP-20 as cathode and MnO_2/AC as anode exhibited energy density of 88.12 Wh kg^{-1} (~1.6 kW kg^{-1}) and cyclic stability of 89.68% for 10,000 cycles. Further, the real-time applicability of the device was tested by illuminating a 39 red LED panel for 45 minutes. The results suggest promising response of ternary composite for hybrid supercapacitors.

k0054

Vanadium doped SnO_2 synthesized using photo irradiation technique: Application as LIB anodes

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Although graphite is most widely used anode material for Lithium-Ion Batteries, it has some limitations regarding its practical applications in high energy and high-power devices because of its very low specific capacity. Alloy type materials have been studied to have appreciably high specific capacity as compared to graphite and other carbon-based

anodes. SnO2 is a very promising conversion alloy type anode material. However, it has a major drawback of pulverization during the lithiation-delithiation process. Herein, we study the improvement in the electrochemical performance of SnO2 as an anode material in LIB, when we dope it with vanadium (V) ions. After 50 cycles, we see an improvement of 80% in specific capacity in case of the 1% V doped SnO2 as compared to the pristine one.

k0055

Investigation of Thermoelectric Properties of Flexible Copper Iodide Thin Films

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P-type Copper Iodide (CuI) is a material that demonstrates potential use in thermoelectric devices. In this study, p-type CuI thin film is synthesized by the I_2 vaporization technique. Iodine vaporization on copper thin film provides an effective and controlled deposition of CuI on paper substrate. This method demonstrates a viable approach for producing high-quality thin films with desirable electrical and optical properties. CuI thin films are synthesized by vaporizing I_2 for 1-hour and 10-hour. The obtained 1-hour and 10-hour vaporised thin film samples exhibit excellent conductivity of 700 S m^{-1} and 1800 S m^{-1} and thermopower of 90 µV K^{-1} and 70 µV K^{-1}, resulting in power factor of 5.7 µW m^{-1} K^{-2} and 9 µW m^{-1} K^{-2} in 1 hour and 10-hour I_2 vaporized thin film, respectively. The power factor of 10-hours vaporized thin film is higher than 1-hour vaporized film. This synthesis method provides a versatile and reproducible process and also gives possibilities for further optimization of CuI-based materials for advanced technological applications. This study illustrates the possibility of CuI as an important material in advancing the efficiency of thermoelectric systems.

k0057

Optical Properties of WO_3 and WO_{3-x} Nano-structured Photoanodes for Electrochemical Water Splitting

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Oxygen deficiency in tungsten oxide (WO_{3-x}) gives rise to mid-gap defects states near the conduction band minima. Prolonged carrier lifetime arising from electrons in these defect states enhances the charge transfer rate, which plays a key role in enhancing the photo electrochemical (PEC) catalysis performance. In view of these, we present here a comparative study of photoelectrochemical, structural and optical properties of commercial WO_3 powder, WO_3, and WO_{3-x} nanostructures. Formation of shallow donor states in WO_{3-x} lowers the optical bandgap from 2.7 eV to 2.59 eV: as is evident from UV-Vis spectroscopy. The presence of W^{+5} oxidation state in WO_{3-x} along with stoichiometric WO_3's W^{+6} state, as noted from XPS data, confirms oxygen-deficiency in this nano material. The structural changes brought about by this lattice oxygen deficiency are further evident from Raman spectra and x-ray diffraction analysis. The nanosheet morphology and crystalline nature are noted from transmission electron microscopy. The charge transfer resistance in WO_3 nanosheets is found to have lowered compared to commercial powder in the EIS measurements. Finally, PEC studies on WO_3 are presented with and without light illumination, and also with UV and Vis light filters.

k0058

A First-Principles Study of Structural and Electronic Properties of 2-Iodoethylammonium Lead Iodide Perovskite

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Abstract. The rapid enhancement in efficiency of solid-state solar cells has brought particular focus to hybrid organic–inorganic halide perovskites because of their high photovoltaic efficiency. Our research entailed first-principles calculations to explore the crystal structures, as well as the electronic properties of 3D organic-inorganic hybrid lead

iodide pervoskite $[I(CH_2)_2NH_3]_2PbI_4$. The material also exhibits magnetic properties attributed to carbon atoms, offering opportunities for novel device concepts. Our calculations reveal a direct energy band gap of 1.935 eV in the down-spin channel, suggesting potential for solar energy harvesting. The calculated crystal structure parameters are in reasonable agreement to the experimental values. The results approve that these compounds could be promising materials for spintronic and optoelectronic devices.

k0059

Influence of Humidity on ZnO based Triboelectric Nanogenerator

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This study explores the effect of humidity on contact electrification, continuing in the principle of the triboelectric effect. Specifically, it examines how the adsorption of moisture impacts the efficiency of triboelectric nanogenerators (TENGs) and charge transfer in the materials. TENG based energy generation is poised to be the next significant advancement, high-humidity regions raise a problem in the efficiency of the generator. The research focuses on the contact electrification of ZnO with various counter layers, both hydrophobic and hydrophilic, in a controlled humid chamber. Further, the study investigates the use of a PVA-layered ZnO to mitigate the impact of humidity on contact electrification.

k0060

Development of Ni-N Coatings for Electrocatalysis

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Electrocatalysis is an efficient and promising means of energy conversion. To enhance reaction rates, catalysts are required to minimize the overpotential. In this context, in recent years, transition metal nitrides (TMNs) are getting a lot of attention owing to their high catalytic activity, distinctive electronic structures, and enhanced surface morphologies. Among TMNs, nickel nitrides (Ni-N) are emerging as an ideal choice for electrocatalysts due to high abundance and low cost of Ni in comparison to established noble metal based electrocatalysts. Different phases of Ni-N can be formed by varying the N concentration. We deposited a series of Ni-N coatings by varying the nitrogen partial pressure (RN2) at 0, 15, 50, 75, and 100% (rest Ar) in the reactive sputtering process. It was found that N atoms get incorporated in Ni, leading to formation of Ni3N phase at RN2 = 100%. The oxygen evolution reaction (OER) measurements were performed on Ni-N films and it was found that the overpotential get suppressed substantially in Ni3N as compared to pure Ni films. It is foreseen that Ni-N based coatings can be further developed by suitably varying the deposition parameter to realize noble metal free electrocatalysts.

k0061

Effect of $LaNbO_4$ coating on $LiNi_{0.88}Mn_{0.06}Co_{0.06}O_2$ cathode materials for high performance lithium-ion batteries

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$LiNi_xMn_yCo_zO_2$ (NMC) cathodes have a significant impact on energy storage applications, but with several degradation drawbacks. Metal oxide coating is the most direct and effective solution to alleviate this material degradation. In this work, we present an integrated $LaNbO_4$ (LN) surface coating strategy for improving $LiNi_{0.88}Mn_{0.06}Co_{0.06}O_2$'s (NMC-88). The rietveld refinement supports the identification of the phase and crystallinity of the material. The coating elements protect the cathode surface from unwanted side reactions. After 150 cycles at 2C, the modified cathode retains 42% more capacity than the pristine NMC-88 cathode. Compared with NMC-88, the enhanced electrochemical performance and structural integrity of LN-coated NMC-88 are correlated to the reduction of microcrack defects during cycling.

k0064

Impact of Heat Treatment on Phase Formation and the Transport Properties of $AgSbTe_2$ Thermoelectric Materials

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In the current study, we have investigated the intrinsic thermodynamic metastable phase of $AgSbTe_2$ and its influence on the electrical and thermal properties. The bulk polycrystalline material of $AgSbTe_2$ was synthesized by the solid-state reaction technique via vacuum encapsulation techniques. The room temperature XRD data show the presence of $AgSbTe_2$, Sb_2Te_3, and Ag_2Te phases in the studied samples, confirming the metastability of $AgSbTe_2$. The temperature dependent resistivity study verified the cationic disorder arrangement in the material. Hall measurement at room temperature showed p-type conductivity. Our study demonstrates the studied material's phonon-glass electron-crystal (PGEC) behavior, a critical property for its thermoelectric performance.

k0066

Harnessing the Potential of MOF-74 (M = Co, Ni, Cu) for Enhanced Water Splitting Reactions

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Exploring cost-efficient catalysts with bifunctional activities of hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) holds practical significance for overall water splitting. Hydrogen (H_2) is a promising option due to its high energy density and environmentally friendly combustion, producing only water. However, efficient and cost-effective H_2 production remains challenging. Metal-organic frameworks (MOFs), with their high surface area and tunable properties, offer a viable solution. In this study, MOF-74 materials with cobalt, nickel, and copper metal centers were synthesized via a solvothermal method, characterized, and evaluated as electrocatalysts for hydrogen production from water splitting. The polarization curves showed a similar onset potential for the OER, achieving 10 mA/cm² at 2.35 V. For the HER, Co-MOF-74 exhibited the highest activity, with an over potential of 0.21 V at 10 mA/cm².

k0068

Comparative study of $Y_2Sn_2O_7$:Eu and $La_2Sn_2O_7$:Eu phosphor

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In this work, comparative photoluminescence study have been carried out on $Y_2Sn_2O_7$:Eu and $La_2Sn_2O_7$:Eu phosphor. In line with radius ratio (r_A/r_B) rule, powder XRD analysis indicates pyrochlore phase (*Fd3m*) formation of both the oxides. Photoluminescence (PL) of both the ternary oxides exhibits dominant magnetic dipole transition ($^5D_0$-$^7F_1$) at ~590 nm in comparison to electric dipole transition ($^5D_0$-$^7F_2$) at ~610nm, indicating the occurrence of symmetric EuO_8 polyhedra which is justified with pyrochlore structure. Though, both oxides have pyrochlore structure, but the local symmetry around the probe ion (i.e., asymmetric ratio I_{610}/I_{590}) in the two system is quite different suggesting the difference in their local structure. The variance in local symmetry was also manifested in the decay lifetime of $^5D_0$ level of Eu.

k0069

Vibrational and thermodynamic properties of $K_2Ni_2TeO_6$

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Abstract: $K_2Ni_2TeO_6$ is a two-dimensional layered battery material, consisting of alkali atoms sandwiched between slabs exclusively made of transition metal atoms arranged in a honeycomb fashion. The vibrational and

thermodynamic properties of this material was investigated using potential model calculations. The reported specific heat data are in good agreement with calculations.

k0070

Study on Electrochemical Performance of Glass-Ceramics Based Composite Solid Electrolyte for Lithium Battery

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Commercial liquid electrolyte makes conventional lithium batteries unsafe in terms of flammability. Solid state electrolyte may ensure the improvement over the safety issues. In this study, we report the synthesis of Composite Solid Electrolytes (CSEs) using different weight percent of NASICON-type $Li_{1.25}Al_{0.5}Ge_{1.5}P_{2.75}Mo_{0.25}O_{12}$ (LAGPM) glass ceramics (GC) solid electrolyte along with two suitable polymers. The value of d.c. ionic conductivity of LAGPM is 4.93×10^{-4} Scm^{-1}. TGA analysis shows that the prepared CSEs are thermally stable upto 450°C. The thickness of the CSEs is ~60µm. Among all the prepared CSEs, the sample containing 60wt% of LAGPM (LAGPM60) possesses the highest quantity of amorphous region. Fabricated solid state cell using LAGPM60 shows a stable specific discharge capacity of 140mAhg^{-1} at the current rate of 1C (=170mAg^{-1}) upto 100cycles.

k0071

Optimization of Potential Window for PPy/PVA based Electrode Material for Supercapacitor Applications

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With the rising human population, the demand for energy is continuously escalating, constrained by the finite availability of non-renewable energy sources. Consequently, the interest in renewable energy sources is increasing. However, these sources, including wind, solar, and thermal energy, are highly location-dependent. This has led to a growing need for efficient energy storage devices such as batteries, fuel cells, and Supercapacitors. Among these devices, Supercapacitors are particularly notable for their rapid charge-discharge capabilities. Nevertheless, their practical application is limited by their relatively low energy density. The energy density of a Supercapacitor directly depends on the specific capacitance and the square of potential window. In this research, we have synthesized a binary composite of PPy/PVA via in-situ polymerization reaction and characterized it using X-ray diffraction. The electrochemical measurements were performed on a 3-electrode setup using 1 M H_2SO_4 as an electrolyte. To maximize the energy density, specific capacitance was optimized by optimizing the potential window of composite using CV and GCD measurements. The potential window of the composite was optimized to be 1.2 V with a value of specific capacitance as high as 1197 F/g at 10 mV/s demonstrating its capability to be used as an electrode material for future Supercapacitor applications.

k0072

Characterization Of Interface Between Lipon Solid Electrolyte And Tio_2 Anode Of Lithium Ion Battery By Spectroscopic Ellipsometry

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Magnetron sputter deposited amorphous thin film of Li3+xPO4-xNx (LiPON) solid state electrolyte and LiPON/TiO2 (anode) thin film bi-layers have been characterized by spectroscopic ellipsometry to study the properties of electrolyte-anode interface of Li ion solid state battery. Initially 5 LiPON single layer thin film samples have been deposited on glass substrates at different process conditions following which 5 bi-layer samples of LIPON on top of TiO2 thin film have been deposited on glass substrates maintaining similar process conditions. Subsequently spectroscopic ellipsometry measurements have been carried out on the single layer LiPON and LiPON-TiO2 bilayer thin film samples. Using the single layer ellipsometry data optimized process conditions for deposition of LiPON films have

been obtained and the using bi-layer ellipsometry data electrolyte-anode interfaces have been studied non-destructively.

k0074

Structural, Impedance and Modulus Study of Mg Doped Cobalt Ferrite for Energy Application

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Spinel ferrites, particularly cobalt ferrites having a reverse type spinel morphology, are crucial for applications in information storage systems, sensor-based devices, telecommunication systems, and microwave absorbers. This study examines the structural parameters using XRD, as well as impedance, and modulus properties of $CoFe_2O_4$ doped with magnesium. Results show distinct peaks indicating grain and interface relaxation processes, with temperature-dependent variations, confirming the material's suitability for advanced applications.

k0078

$MoTe_2/Ti_3CN$ Based Composite for Efficient Hydrogen Evolution Reaction

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Addressing the global energy crisis and environmental degradation necessitates the development of efficient and sustainable hydrogen production methods. Water splitting is a promising technique, yet achieving long-term hydrogen production requires cost-effective and durable electrocatalysts. Conventional platinum-based catalysts, despite their effectiveness, are expensive and limited in supply. This study investigates the potential of a composite comprising $MoTe_2$ and Ti_3CN MXene as an alternative. The $MoTe_2/Ti_3CN$ MXene composite exhibits exceptional hydrogen evolution reaction (HER) performance, with a notably low overpotential and Tafel slope, surpassing the performance of the individual components. Additionally, the composite demonstrates excellent stability, maintaining its catalytic activity after prolonged cycling. These findings suggest that the $MoTe_2/Ti_3CN$ MXene composite not only enhances HER efficiency but also offers a cost-effective and durable alternative to platinum-based electrocatalysts, making it a promising candidate for sustainable hydrogen production.

k0079

Mixed Dimensional WS_2/WSe_2 Heterostructure for Optoelectronic Application

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Two-dimensional semiconductors have good carrier transport and strong light-matter interaction, making them intriguing candidates for next-generation optoelectronics. The TMDCs based hetero-structures is becoming fascinating breakthroughs in increasing optoelectronic characteristics. Therefore in the present work, we investigated the optoelectronic properties of 2D nanosheets/1D nanorod mixed dimensional WS_2/WSe_2 heterojunction diode. Raman and elemental studies conform to the hexagonal crystal strucuture and their corresponding elements are presented. The I-V characteristics of the device is measured under the absence and presence of the light. The calculated ideality factor and rectification ratio are 1.04 and 6.07 under illumination of the light. The numeraical simulation studies shows the WS_2/WSe_2 behaves like typical photodetector. These fundamental studies provides the advances of WS_2/WSe_2 van der waals heterostructures in photodiode and solar cell applications.

k0082

Higher Manganese Silicide by Molten Salt Shielded Synthesis Method

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Silicides are considered as one of the potential candidates for commercial thermoelectric applications, as they are non-toxic, stable and made up of earth abundant elements[1,2]. Mg_2Si, $MnSi_x$, $CrSi_2$, and β-$FeSi_2$, are some of the silicides studied for thermoelectric applications. Among these silicides, $MnSi_x$ show good thermoelectric performance at mid-

temperature range with good mechanical stability. In this work we have synthesized $MnSi_x$ with excellent thermoelectric properties by a cost-efficient molten salt shielded synthesis method[3] in atmospheric condition. This method overcomes the difficulties in the conventional methods such as arc melting, ball milling, hot pressing, chemical vapor transport and spark plasma sintering that requires high temperature and vacuum[4]. The synthesized silicide samples have been sintered by spark plasma sintering. The phase, morphology and elemental composition of the synthesized materials have been characterized through X-ray diffraction, scanning electron microscopy and EDX. The Rietveld refinement of diffraction pattern confirms the formation of higher manganese silicide along with a minimal MnSi impurity phase.

k0083

Synthesis and Characterisation of δ-MnO_2 for High Performance Supercapacitor Electrode Application

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High-capacitance manganese dioxide (δ-MnO_2) nanoparticles were synthesized via a co-precipitation method for supercapacitor electrode applications. The obtained δ-MnO_2 was characterized using X-ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), and Scanning electron Microscopy (SEM), confirming its successful synthesis. Electrochemical evaluations, including Cyclic Voltammetry, Galvanostatic Charge Discharge, and Electrochemical Impedance Spectroscopy, demonstrated a specific capacitance of 220 Fg^{-1} at 1 Ag^{-1}. These findings underscore the potential of δ-MnO_2 as a highly effecient electrode material for supercapacitors.

k0084

Exploration of Potential Solid-State Fluoride Ion-Conducting Electrolyte - $PbSnF_4$

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Solid state Fluoride ion batteries are emerging post-lithium technology mainly due to their high energy density. The main challenge for designing potential fluoride ion batteries is to develop a suitable solid electrolyte with high ionic conductivity. As the superionic ternary material PbSnF4 is the most conductive fluoride ion conductor among all known materials, the present work focuses on the microstructural, morphological, and transport properties of nanocrystalline PbSnF4. The monoclinic (α phase) structure of PbSnF4 synthesized using sonochemical technique has been explored as a promising high-performance solid electrolyte for fluoride ion batteries. As the synthesis route directly impacts the material's microstructure and morphology, enhancing its ionic transport properties, the simple and economic sonochemical strategy is employed in this investigation. Impedance spectroscopy was used to investigate the room-temperature ionic conductivity of the synthesized α-PbSnF4. The PbSnF4 synthesized via the sonochemical method exhibits an ionic conductivity of 5.9×10-4 S/cm at room temperature with an ionic transference number 0.88 as revealed by the DC polarization studies.

k0089

Evidence of Fission Gas Bubble in High Burnup Er and Sn Nuclear Target

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The MeV-range energetic ions beyond Coulomb's barrier of a target-beam combination lead to nuclear reactions, subsequently the modification of target materials. The reaction yields are energetic and produce local heat as inelastic in nature and give up energy to the matrix around. In the traversing path there will be direct collision and successive collision cascade due to lattice displacement. The LWR and AGR fuel behavior in the reactor environment is essential and complicated and feedback understanding of the spent fuel or similar type studies impart more understanding of

the material degradation. In this study we have reported the High burn up structure (HBS) of targets Er and Sn exposed to 180 MeV Si and 30 MeV Li io using 15 UD Pelletron accelerator respectively via SEM and XRD.

k0091

Synthesis of highly efficient WS_2 and WSe_2 electrocatalyst by simple chemical method

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Green and sustainable energy sources play a pivotal role in meeting the rapidly growing global energy demand and consumption. The catalysts with surface-active sites are prime concerns in the design of new and efficient catalysts/electrode materials for electrochemical energy conversion and storage systems. Here, we present the low-cost preparation method for synthesis of 2H hexagonal WS_2 and WSe_2 stable, and efficient electrocatalysts for hydrogen evolution. The chemical synthesis method yields nanosheets with high density of active sites for both WS_2 and WSe_2 semiconductors. It is observed that the WSe_2 catalysts show better HER performance, recorded a 300mV. vs RHE overpotential at mA/cm^2 current density in 1MKOH electrolyte.

k0094

$MAPbI_3$ Perovskite Surface with an Extravagant Structural Arrangement Through the Integration of 2-amino Benzothiazole for a Long-lasting and Efficient Solar Cell

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The poor long-term stability of $MAPbI_3$ perovskite in light, heat and humid environments is a major obstacle to commercialization. Degradation of $MAPbI_3$ and an impairment in non-radiative charge recombination, a major impediment to increasing the stability and efficiency of photovoltaic devices, are made possible by the trap state and surface imperfections between the perovskite and ETL interfaces. Here, the surface defect was healed 2-amino benzothiazole (Lewis's base) by activating the heteroatoms of S and N and the amine functional group for defect passivation. In the context of defect passivation, systematic investigation is conducted on forming hydrogen bonds between N—H—I or the coordination between uncoordinated Pb^{2+} and heteroatoms of S and N. A high photovoltaic efficiency of 21.5% with improved V_{oc} and FF was demonstrated with the optimum concentration of passivating material (2 mg/ml IPA) than the pristine $MAPbI_3$ PCE of 19.4%. As shown by stability studies, the 2-ABT integrated device outscored the pristine $MAPbI_3$ device, retaining 87% of its PCE after 500 hours in N_2.

k0095

Methyl Orange Dye Decomposition By Tio_2 Nano Particles: Optimization And First Order Langmuir–Hinshelwood Dynamics

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The study uses a cost-effective co-precipitation method to produce well-crystalline pure TiO_2 and Fe-doped TiO_2 (Fe-TiO_2) nanoparticles with a loading concentration of 4 mol% Fe at 400°C calcination temperature. The structural and microstructural characterization is examined using Powder X-ray diffraction and emission electron microscopy. Results show Fe-TiO_2 NPs have tetragonal structure with almost spherical morphology. The doping amount of Fe significantly affects the crystalline size and Fe-TiO_2 nanocrystals' activity as catalyst. The modified Fe-TiO_2 (of average size 76 nm) nano catalyst exhibit significantly higher photocatalytic activity than pure TiO_2 NPs (of average size 100 nm) under visible and ultraviolet light photoreactors. Fe-TiO_2 nanocatalyst has a maximal degradation efficiency of 60% under Vis-L in 7.5 hours compared to undoped catalysts which degrades 45% in 24 hours. Injecting Fe ions onto Fe-TiO_2-based nanocrystals results a rapid 75% degradation under UV assistance making TiO_2

photocatalyst more versatile. According to Langmuir-Hinshelwood dynamics the degradation of Methyl Orange (MO) dye follows the pseudo-first-order kinetics for the entire as-synthesized nanocatalysts.

k0096

Enhanced Thermoelectric performance of 2D VSeTe via Strain Engineering

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Strain-engineering has emerged as a powerful and efficient technique for modulating the physical properties of two-dimensional (2D) materials, including their thermoelectric coefficients and lattice thermal conductivity. In this study, we investigate the thermoelectric properties of VSeTe monolayers under biaxial compressive and tensile strains using first-principles calculations and the Boltzmann transport equation. Analysis of the elastic constants and Poisson ratio confirms the applicability of strain, while phonon dispersion curves reveal the dynamical stability of the proposed structure. Our results demonstrate that strain engineering significantly impacts the electronic band structure. Specifically, biaxial tensile strain increases the Seebeck coefficient and reduces lattice thermal conductivity, resulting in an improved figure of merit (ZT). At room temperature, the figure of merit for p-type doping reaches 2.47 under 2% tensile strain, representing an almost 8-fold increase compared to the unstrained value of 0.308. These findings highlight the potential of tensile strain to significantly enhance the thermoelectric efficiency of VSeTe monolayers, making them highly promising for thermoelectric device applications at room temperature.

k0099

Temperature-Dependent Electrical Conductivity And Relaxation Dynamics In PVDF/MWCNT@$BaTiO_3$ Polymer Nanocomposites

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Polymer Nanocomposites Comprising of PVDF/MWCNT@$BaTiO_3$ were studied. The structural, microstructural and thermal properties were confirmed from XRD,TEM, and DSC/TGA datas respectively. The proper distribution of Core-shell nanoparticles in PNC are also confirmed from FESEM/EDAX datas. Phase transitions as well as Tg value of PVDF shifts toward room temperature with varying frequency due to coating of $BaTiO_3$ ceramic fillers confirmed from dielectric results .The Modulus spectroscopy confirms a non-Debye type universal relaxation behaviour (β=0.57 to 0.74) for the temperature above 350K attributed due to the interfacial polarization. Due to complex dielectric behaviour and low loss tangent~0.1 may be suitable for charge storage application.

k0100

CdSe Quantum Dot Synthesis and Application in Quantum Dot Dye Sensitized Solar Cell

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Using a safe procedure, Cadmium Selenide (CdSe) quantum dots(QD's) were synthesized by wet chemical method. The synthesized CdSe QD's are characterized by XRD (X-ray diffraction) ranging QD's size from 1.9 nm to 6 nm, SEM (Scanning Electron Microscopy), UV-Visible Spectra (UV-Visible Spectroscopy), and FTIR (Fourier Transform Infrared Spectroscopy). In the application part, to calculate the efficiency of solar cell electrodes, we used the PEC (Photoelectrochemical cell) three-electrode set-up for characterization and Cyclic Voltammetry to check the capacity of the electrode. Using a CdSe material, we have prepared the electrode on ITO with the help of the Drop Cast method, which shows efficiency 1.240 % by PEC test.

k0101

Electrochemical Properties of $Co_{0.5}Cu_{0.5}Fe_2O_4$/PANI Nanocomposites for Energy Storage Devices

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In this work we report the fabrication of $Co_{0.5}Cu_{0.5}Fe_2O_4$ ferrite nanoparticles by sol-gel auto-combustion method. $Co_{0.5}Cu_{0.5}Fe_2O_4$ /Polyaniline nanocomposite was prepared by in-situ polymerization method. Prepared samples were characterized by XRD and FEG-SEM. The material's capacity to store charge and its dependability as an active electrode have been proven using a traditional three-electrode approach. $Co_{0.5}Cu_{0.5}Fe_2O_4$ nanoparticles and nanocomposite shows electrochemical energy storage performance with a specific capacity of 27.1 Fg^{-1} and761 Fg^{-1} at a scan rate of 5 $mVsec^{-1}$. The electrochemical energy storage performance increased due to polyaniline.

k0102

Correlating Structure And Functionality of $KBiFe_2O_5$ With XRD, Raman, UV-Visible And FT-IR Spectroscopy

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KBiFe2O5, a fascinating Brownmillerite material, has captured the interest of researchers not only for its multiferroic properties, but also for its potential in the realm of photovoltaics. While KBiFe2O5 possesses some inherent light-harvesting capabilities, researchers are exploring ways to optimize its performance for solar energy conversion. In this study, we investigated the structural, vibrational, and functional properties of KBiFe2O5 using a combination of X-ray diffraction (XRD), Raman spectroscopy, UV-Vis and Fourier-transform infrared (FTIR) spectroscopy. We synthesized the material via solid state route and Samples were calcined at the temperature 750°C. Rietveld refinement shows the material is a monoclinic with space group P2/c at the room temperature. Tauc-plot shows that the sample has bandgap of 1.8 eV. Characteristic phonon modes in FTIR suggests KO, Fe-O and Bi-O interactions. Raman spectra suggest collective motions of the crystal lattice, resulted in broad bands, particularly in the lower frequency region.

l) 1-D, 2-D AND QUANTUM MATERIALS

l0001

Synthesis of MoS_2 Thin Films from Bulk-like to Monolayer and Their Valence Band Offset with SiO_2 Interfaces

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This study presents the synthesis of MoS_2 thin films ranging from few layers to monolayers and their band offset with SiO_2 interfaces. MoS_2 thin films were synthesized using e-beam deposition followed by sulfurization on SiO_2/Si substrates. Grazing incidence x-ray diffraction (GIXRD) confirmed the formation of the 2H phase. The valence band offset (VBO) at the MoS_2/SiO_2 interfaces were investigated using x-ray photoelectron spectroscopy (XPS). The VBO were measured and found to be sufficient (>1.0 eV) to suppress gate current, indicating the potential of MoS_2/SiO_2 heterojunctions for high-performance field-effect transistors (FETs) and photodetectors. The results contribute to the understanding of MoS_2-based nano-electronic devices, highlighting the importance of precise control over film thickness and interface engineering.

l0004

Existence of Phonon Topology in V_3Sn Compound with Six-fold Band Degeneracy: A DFT Study

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The discovery of topological states with multiple-fold band degeneracy has revolutionized our understanding of matter phases and emerged as a leading area of research in condensed matter physics. The inclusion of novel quantum theories such as Berry phase and pseudospin into phonon systems provides new methods for phonon control and give rise to the emerging field of "topological phononics". The phononic systems have the symmetry protected topological phonon transport in the materials. In the present work, we investigated phononic topological phenomena in V_3Sn compound using density functional theory. The phonon dispersion curves confirm the phononic nodal point having six-fold degeneracy at the R high-symmetry point along with three-fold crossing point at the Γ-point. The topological surface spectrum obtained from tight-binding model generated using WannierTools further validates the obtained results. The six-fold degeneracy is maximum fold observed in phonon topology till date. We believe that rich phonon points observed in synthesized V_3Sn have potential applications in phonon waveguides and further drives the experimental realization.

l0005

Local Structural Investigations of Fe Doped Graphitic ZnO and Reduced Graphene Oxide Composite

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This study investigates the electronic structure and local coordination environment of Fe-doped graphitic ZnO (gZnO) through X-ray Absorption Near Edge Structure (XANES) and Extended X-ray Absorption Fine Structure (EXAFS) analysis at the Fe K-edge. Key spectral features, such as the pre-edge and absorption edge, indicate that Fe ions predominantly adopt a +3 oxidation state within the ZnO matrix. Polarization-dependent XANES measurements reveal distinct in-plane and out-of-plane electronic environments, particularly pronounced in the 2% Fe-doped sample. The XANES simulations, assuming a model of stacked graphitic ZnO monolayers with Fe substitutions, closely match the experimental data, validating the layered structural model. Fourier transform EXAFS spectra indicate preferential orientation of the gZnO layers in-plane to the substrate. These findings provide comprehensive insights into the structural and electronic properties of Fe doping in gZnO, with significant implications for the development of ZnO-based materials in advanced technological applications.

l0006

Piezoresistive Pressure Sensors Based On Cellulose Paper Coated With MoS_2 Nanosheets

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Piezoresistive pressure sensing of MoS_2 nanosheets coated cellulose papers were demonstrated. X ray diffraction pattern of MoS_2 nanosheets, exfoliated from bulk powder through ultrasonication, revealed increased interlayer gap between the nanolayers, indicating weakening of van der Waals forces between the layers due to layer thinning. Raman spectra of MoS_2 nanosheets showed blue shift in peak position, compared to that of bulk MoS_2, possibly due to layers thinning and excess Sulphur in nanosheets. Pressure sensors fabricated by stacking MoS_2 coated cellulose papers between two copper plates showed nearly linear increase in response (current/resistance change across cellulose papers) for applied pressure of around 200 – 2000Pa. Sensitivity of these pressure sensors were found to be higher than that using cellulose papers without MoS_2 coating. This is attributed to the atomically thin layered nature of MoS_2 nanosheets which could be causing improved contact between the nanosheets and hence allowing efficient charge transport across the cellulose papers. Since cellulose papers are flexible, these pressure sensors can find applications in wearable electronics and robotics.

l0008

Electron-Phonon Coupling in Interlayer Phonon Modes of $MoSe_{1.8}S_{0.2}$ at Low Temperatures

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Layered materials like metal-dichalchogenides (TMDCs) are studied extensively due to their potential technological applications. Here, we report the Raman spectroscopic investigation of single crystalline dichalchogenide $MoSe_{1.8}S_{0.2}$ at low temperatures. We observed an interlayer mode of $MoSe_{1.8}S_{0.2}$ in the ultra-low frequency range at around 27 cm^{-1} which was not reported so far for this composition. The polarized Raman measurements at room temperature indicates that the symmetry of this mode is E_{2g}. Anomalous behavior of this phonon mode at low temperatures in $MoSe_{1.8}S_{0.2}$ shows electron- phonon coupling at low temperatures.

l0009

Photocatalytic Degradation of Methyl Orange Using Borophene/TiO_2 Quantum Dots Nanocomposite Under UV Light Irradiation

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In this study, the photocatalytic activity of TiO_2 quantum dots (QDs) was improved by synthesizing a nanocomposite with borophene (BP). BP/TiO_2 QDs nanocomposite was successfully synthesized using the hydrothermal method followed by the confirmation through TEM and UV-Vis absorption spectroscopy measurements. The degradation of methyl orange was carried out using both TiO_2 QDs and BP/TiO_2 QDs nanocomposite photocatalysts under UV light irradiation. The result indicates that the dye degradation was more efficient with the BP/TiO_2 QDs nanocomposite than pure TiO_2 QDs. This study presents a novel approach to enhancing the photocatalytic performance of semiconductor photocatalysts in the removal of the organic pollutants.

l0011

Exploration of Hydrogen Decorated Two-dimensional Graphullerene: a First Principle Investigation

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Abstract: We have systematically studied a two-dimensional (2D) structure of hydrogen decorated graphullerene. We employed an ab initio calculation to examine its structural and electronic properties. Graphullerene is a newly discovered 2D allotrope of carbon which is formed by the use of C_{60} crystal of carbon allotrope. We computed structural and electronic band structure of hydrogen decorated graphullerene, which can be a good replacement for

futuristic devices specially for optoelectronic devices due to direct energy band gap (2.74 eV). Which lies in the visible region. It can also be used as hydrogen storage device in the future.

l0012

Investigation Of Structural, Morphology, Thermal, And Magnetic Properties Of $Ni_{0.90}Cu_{0.10}Te_2$ Single Crystal

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Layered Transition Metal Dichalcogenides (LTMDCs) are quasi-two-dimensional materials with notable structural and magnetic properties. Recent research has highlighted intriguing features in the $NiTe_2$ system, especially in LTMDCs. In this study synthesized $Ni_{0.90}Cu_{0.10}Te_2$ using the self-flex technique to explore the effects of Cu doping on NiTe2's structural, morphology, thermal, and magnetic properties. X-ray powder diffraction (XRPD) confirmed a trigonal structure with CdI2-type configuration and a *l*3*m*1 space group, validating the crystalline organization. Field emission scanning electron microscope (FESEM) imaging illustrated the layered structure due to Cu doping. Thermal analysis via thermogravimetry differential thermal analysis (Tg/DTA) demonstrated stability up to 800 °C, with only a 2% weight loss between 800 and 1000 °C. Magnetization studies in a 1 T field showed paramagnetic behavior across 2 to 200 K temperatures. These findings indicate that Cu doping significantly enhances the magnetic properties of $NiTe_2$, making it suitable for magnetic device applications.

l0013

First-Principles Study of Optoelectronic and Photocatalytic Properties of Two-Dimensional $AlAs/SbI_3$ van der Waals Heterostructure

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Using first-principles calculation, we investigated the optoelectronic and photocatalytic properties of two-dimensional (2D) $AlAs/SbI_3$ van der Waals (vdW) heterostructure. The thermal stability of $AlAs/SbI_3$ is characterized in terms of ab initio molecular dynamics (AIMD) simulations, which indicates it is highly suitable for practical implementation in experiments. The $AlAs/SbI_3$ heterostructure possesses an indirect bandgap having a value of 1.63 eV (1.19 eV) at the HSE06 (PBE) level of theory with optical absorption spectra lying in the visible region. Furthermore, the $AlAs/SbI_3$ heterostructure properly engulfs the redox potential of water with a type-II scheme. Thus, due to its semiconducting nature, visible region absorption spectra and proper band alignment make $AlAs/SbI_3$ heterostructure a promising candidate for futuristic optoelectronic and photocatalytic water-splitting field.

l0015

Structural and Magnetic Properties of $FePS_3$ Single-Crystal

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The layered 2D transition metal tri-chalcogenide $FePS_3$ has attracted significant interest owing to potentially diverse candidates for nanoelectronics devices. The structural and magnetic properties of $FePS_3$ have been reported. The X-ray diffraction confirms the presence of monoclinic crystal symmetry with space group C/2m. The electronic structure has been studied using X-ray photoelectron spectroscopy measurement. The XPS analysis confirms the oxidation state of iron (2+, 3+) and spin-orbit coupling in the system. Magnetic property suggests that the $FePS_3$ exhibits a long-range magnetic ordering below 119 K and a glassy state at around 30 K.

l0016

Tunable Electronic Properties of Dirac Cone Square Tellurene(σ-Te_2)

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In this study, we conduct first principles calculations using density functional theory on σ-Tellurene (σ-Te_2). σ-Tellurene is characterized as a Dirac cone material with a Fermi velocity of 9.4×10^5 m/s^{-1}. However, its lack of a

band gap limits its utility in conventional electronics. Our work aims to induce a band gap by applying strain and introducing spin-orbit coupling (SOC) effects. Our findings demonstrate that biaxial strain in conjunction with SOC effectively modulates the band gap, resulting in a significant band gap opening (~0.3 eV) at a biaxial strain of 6%. Importantly, the Dirac cone structure remains preserved. A Dirac cone with a narrow band gap holds promising potential for future applications in electronics, electrochemical devices, strain sensors and beyond.

l0017

Two-dimensional van der Waals Electrical Contact of Janus MoSSe with Dirac Semi-Metal FeB_2 Monolayer

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In this study, we investigate the structural and electronic properties of a 2D Dirac semi-metal, FeB_2 atop a Janus MoSSe monolayer. The individual characteristics of the layers are well-preserved in the van der Waals (vdW) heterostructure ($MoSSe/FeB_2$). Notably, a low Schottky Barrier Height (SBH) (~ 0.6 eV) is achieved. Additionally, we demonstrate that an external electric field can tune the band alignment of MoSSe with respect to the Dirac cone of FeB_2. At an electric field of around 1 V/Å, the contact transitions to Ohmic, facilitating control over the SBH. This study identifies the $MoSSe/FeB_2$ system as a promising candidate for future nano-devices based on vdW materials.

l0018

Electron and Phonon Hydrodynamics In Graphene

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Phonons are the quantum of lattice vibration energy that behave like quasiparticles. The interacting phonons depict hydrodynamic behavior at low frequencies and extended wavelength limits. Phonon hydrodynamics has become popular because it strongly contributes to electrical properties and heat transport phenomena in crystalline materials like graphene. In the case of phonon hydrodynamics, the phonon-phonon scattering is predominant among boundary, impurity, and defect-mediated scattering. Here, we analytically calculated and compared various thermodynamic quantities like energy density, number density, pressure, and specific heat per particle for both phonon and electron in the hydrodynamics regime for graphene. We have analyzed the specific heat capacity versus temperature for various cases and compared it with the traditional Dulong Petit law and Einstein's theory of specific heat. This results in the electron and phonon contributions to the specific heat dominating over the conventional behavior of metal in the low-temperature region. The fluid behavior of electrons and phonons may also violate the Wiedemann-Franz law for the graphene system.

l0019

Electronic, Mechanical and Electron Transport Properties of 2D Penta-Si_3P_2S Monolayer

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Two-dimensional (2D) materials with pentagonal structures exhibit unique physical properties and hold significant potential for mechanical and thermal applications. We used density functional theory (DFT) and Boltzmann transport theory to study the electronic, mechanical, and electron transport properties of the 2D Penta-Si_3P_2S monolayer. The Penta-Si_3P_2S monolayer exhibits an indirect bandgap of 1.62 eV (2.30 eV) at the GGA (HSE06) level of theory. It possesses high mechanical stability and a high power factor. These findings suggest that the Penta-Si_3P_2S monolayer to be promising candidate for use in electro-mechanical and thermo-electric devices.

l0020

2D Bi_2O_5Te Nanosheets for Sensitive and Fast Response Broadband Visible Light Photodetectors

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Bismuth oxychalcogenide nanosheets (Bi_2O_2X, X = S, Se, Te) in their 2D form, have become promising alternatives for potential applications in optoelectronic devices. One of its most common oxide phases, i.e., Bi_2O_5Te, also possesses quite interesting physical properties, which are yet to be explored. Here, this study reports the photodetectors (PDs) based on 2D Bi_2O_5Te nanomaterial prepared using a "microwave-assisted method," an exciting choice for synthesising such nanomaterials. The basic characterizations confirmed the sample's phase and presence of constituent elements and microscopic studies demonstrated its 2D layered nature. Raman studies confirm different bonds between the atoms. Optical studies represent the band edge of the material around 400nm with band gap of 2.72 eV useful in solar cells, LEDs, and PDs. The broad photoluminescence spectra centers around 650-700 nm, suggesting its optoelectronic applicability. Figures of merits such as sensitivity, responsivity, and detectivity values are obtained from the photodetection measurements, which is quite impressive for fabricating highly sensitive PDs.

l0021

Resistive switching behavior of $MoSe_{2-x}$ nanostructures

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Two dimensional $MoSe_2$ semiconductor known to exhibit interesting catalyst, magnetic and electronic properties. Here, we report the resistive switching behavior of $MoSe_2$ nanostructures including 2D nanosheets and 3D nanoflower. The structural and compositional analysis reveals that the synthesized $MoSe_2$ crystallized into 2H hexagonal crystal structure and possesses Se vacancies. The memristor device made with nanosheets (Au/MOSe2-x-S/Au) and nanoflower (Au/MoSe2-x-F/Au) samples exhibits bipolar asymmetric resistive switching. The nanoflower memristor shows a better-switching performance with ON/OFF ratio of 102 (at 1.5V) and long cyclic stability as compare to the nanosheet memristor.

l0022

High Pressure Structural and Resistance Studies on Type-II Dirac Semimetal $PtTe_2$

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We present high pressure studies of the structural and electrical properties of type-II DSM candidate $PtTe_2$ using synchrotron based x-ray diffraction and resistance measurements up to ~20 GPa. The quasi-two-dimensional ambient trigonal structure remains stable up to 9 GPa above which the system undergoes a structural transition where interlayer van der Waal spacing decreases rapidly, indicating a crossover from quasi-2D to 3D structure at this pressure. The coexistence of the phase separated structures up to the highest pressure of this measurement indicates the first-order nature of this transformation. We also observe an anomalous change in intra-layer atomic rearrangements near 5 GPa, suggesting possible iso-structural electronic (Lifshitz) transition at this pressure. Our low temperature resistance measurements down to 1.8K under quasi-hydrostatic pressure up to ~11 GPa show that PtTe2 remains metallic without the emergence of superconductivity. However, the RRR ($=R_{300K}/R_{2K}$) value systematically increases up to 3 GPa and then starts decreasing rapidly at higher pressures, further supporting the iso-structural electronic transition at this pressure. An abrupt increase of overall resistance above 9 GPa may be due to the structural transition.

l0023

Effect of Residual Oxygen in Atmospheric Pressure Chemical Vapor Deposition growth of monolayer MoS_2

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Abstract. In this paper, we present the effect of residual oxygen on the growth of monolayer MoS_2 in a two-zone atmospheric CVD system. We demonstrate that inadequate atmospheric oxygen removal from the furnace tube, results in either etched MoS_2 flakes or irregular flakes on the substrate, whereas effective removal of atmospheric oxygen

from the tube by purging with high flow of Ar gas, yields monolayer MoS_2 triangular flakes. The as-grown samples were studied with fluorescence optical microscope and Raman spectroscopy.

l0025

Investigation of Fe-B based Two-Dimensional Antiferromagnet for Spintronic Applications

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Antiferromagnetic materials have huge potential for future spintronic applications as they zero net magnetization, unaffected from external perturbation and do not scatter. Here, we explored 2D transition metal boride (MBenes) obtained from bulk layered transition metal boride Fe_2AlB_2 (MAB phase) after removal of Al layer using density Functional theory. Our results show 2D Fe_2B_2 MBene as thermally, mechanically and dynamically stable. 2D Fe_2B_2 found to be antiferromagnetic metal with atomic magnetic moment is 2.33 μ_B/Fe. Furthermore, 2D Fe_2B_2 possess out-of-plane easy axis and the calculated magnetic anisotropy energy is 2.37 meV/atom (U=0 eV) & 38.61 meV/atom (U=5 eV), without and with Hubbard U correction, respectively. The excellent structural stability, robust magnetism and sizeable magnetic anisotropy of Fe_2B_2 monolayer make it promising for future spintronic applications.

l0026

Magnetic properties of the spin-1/2 zigzag chain antiferromagnet: $ZnCuV_2O_7$

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In this study, we have investigated the structural and magnetic properties of 3d9 Cu2+ spin-1/2 one-dimensional (1D) zigzag chain ZnCuV2O7 compound by the combination of x-ray diffraction, dc- and ac-susceptibility, magnetization, and heat-capacity. It has a monoclinic symmetry which is composed of square pyramid CuO5 and VO4 tetrahedra. The bulk measurements such as ac- as well as dc-magnetic susceptibility curves and heat-capacity all together reveal a long-range antiferromagnetic ordering at TN = 3.9 K and a signature of short-range correlations occurs at TSRO ~39 K, as shown by the downward arrow in Fig. (c-f). Moreover, the extracted effective moment from our inverse susceptibility Curie–Weiss fit reveals a nearly divalent Cu2+ ion moment as ~2.0 □B, and a Curie–Weiss temperature was found to be □CW = -40.6 K, confirming dominant interactions are in antiferromagnetic nature. The low-dimensionality nature of magnetic lattice is confirmed by spin-1/2 Bonner-Fisher model fit over magnetic susceptibility which renders nearest neighbor (NN) interaction Jintra ~39.4 K. In addition, the frustration index f = □CW/ TN was found to be ≈ 10.4, suggesting that the magnetic lattice is highly frustrated. Interestingly, the magnetic ordering has been suppressed by the application of a magnetic field at or above 9 Tesla as confirmed by the field-dependent heat capacity [Fig. (f)], indicating that ordered magnetic state can be tuned by an application of applied magnetic field.

l0028

Magnetic properties and possible quantum criticality in Co^{2+} based stacked-honeycomb antiferromagnet: $Ba_2Co(PO_4)_2$

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We have investigated Co2+ honeycomb-lattice $Ba_2Co(PO_4)_2$ compound in which the structure is composed of CoO_6 octahedral environment. The x-ray refinement reveals monoclinic symmetry with space group P 21/n. We have measured detailed thermodynamic properties by means of susceptibility, magnetization and heat-capacity at various applied fields (H). All together suggest that it order antiferromagnetically below TN = 3 K and a pronounced broad maximum at Tmax = 4 K, indicating low-dimensional nature along with short-range correlations are present just above TN. In addition, the extracted Curie-Weiss temperature and frustration index was found to be θCW = −23.1 K and f

= 7.8, respectively, indicating a highly frustrated lattice. Further, magnetization data clearly show a field-induced spin-flop phase transition at Hc = 3 T and an asthmatic trend of saturation develops around an applied field of H = 10 T. Moreover, we have measured 31P NMR to explore the spin dynamics and local structural environment of the complex structure which reveals similar behavior of magnetic spin susceptibility (spin). Interestingly, the LRO is fully suppressed just above an applied magnetic field of 5 T and we have plotted a magnetic phase-diagram in H-T plane which suggests a possible field-induced quantum criticality at HC = 6.5 T as confirmed from extrapolating the phase boundaries of (T) and Cp (T) data. This represents a crossover from the AFM ordered state to the quantum paramagnetic state.

I0029

MoS_2 Nanostructure for Selective Detection of 2,5-Dimethylfuran: A Potential Breath Test Marker for Lung Cancer

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This investigation examines the potential of MoS_2 nanoribbon and nanoflake as gas sensors for detecting volatile organic compounds (VOCs) associated with lung cancer, such as 2,5-Dimethylfuran (C6H8O), using density functional theory (DFT) calculations. Upon adsorption of VOCs, a significant decrease in band gap or HUMO-LUMO is observed, indicating enhanced conductivity suitable for gas sensing applications. The MoS_2 nanoribbon and nanoflake displays particularly strong adsorption energy and a promising sensor response, emphasizing its potential in developing sensitive and selective gas sensors for early lung cancer detection.

I0030

XPS and Structural Characterization of Layered MoS_2 Formed by Thermal Evaporation

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This study presents the synthesis and characterization of MoS_2 thin films prepared by thermal evaporation. XRD patterns confirm the formation of molybdenum disulfide (MoS_2) in the β-2H phase with high crystallinity, while FESEM images illustrate well-stacked layers. X-ray Photoelectron Spectroscopy (XPS) analysis reveals uniform stoichiometry throughout the surface of the film.

I0031

Fingerprints of High Energy Fractionalized Excitations and Spin Jamming in 1-D Antiferromagnetic Spin-1/2 Trimer Chain.

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The study of elementary and composite excitations in highly correlated systems is the most fascinating research field in modern condensed matter physics. However, identifying and studying these excitations are still challenging experimentally. Here, we report Raman spectral signatures of high-energy quasiparticle excitations over a wide temperature range between 80K and 500K of the 1D periodic lattice of antiferromagnetic spin 1/2 chain trimer $Na_2Cu_3Ge_4O_{12}$ (NCGO). The thermal evolution of the integral intensity of the broad spectral background below 170K could be explained considering photon scattering by two fermions excitations. The dynamic Raman susceptibility, as obtained by analyzing the broad spectral background, exhibits the signature of spin jamming at the crossover between fractionalized highly entangled spin states and the normal paramagnetic state in this system.

I0032

Microwave Synthesis of Transition Metal Doped Two-Dimensional Metal Oxide

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Over the past decades the two-dimensional (2D) materials beyond graphene have brought fresh prospects in the field of spintronics, data storage and memory devices. However, the class of layered oxide 2D materials at the nanoscale level has garnered significant attention for their unique electronic, optical, catalytic and magnetic properties. Due to the ultra-thin nature of the 2D metal oxides, a majority of the atoms are available on the surface (high surface-to-volume ratio), which induces new properties and applications as compared to their bulk counterparts. We focus on hematene, which is an atomically thin sheet of Iron (III) oxide derived from its corresponding metal chloride upon microwave irradiation. Here, we doped the hematene atomic sheets with the transition metals to engineer the band gap and the magnetization. The 2D morphology of each of them was confirmed from the high-resolution transmission electron microscopy and the chemical identification was done by X-ray Photoelectron and Raman Spectroscopy. The doped material exhibits both positive and negative photoconductivity under different illuminations and magnetic measurements reveal enhanced ferromagnetic ordering, suggesting its potential for advanced spintronics applications.

l0033

Magnetic Properties of quasi-one-dimensional $BaCo_2Si_2O_7$

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Low dimensional magnetic material has recently grabbed the attention of researcher due to their unique properties. Here, the magnetic behaviour of quasi one-dimensional oxide bridge CoO_4 chained $BaCo_2Si_2O_7$ was studied based on dc-magnetization measurements and low temperature neutron diffraction. X-ray diffraction confirmed single phase nature the compound crystalizes Monoclinic structure. Magnetization data show the compounds orders antiferromagnetically at T_N ~21.5K. Curie-Weiss analysis give θ_P to be ~-48.5 K and μ_{eff} ~ 3.37 μ_B/Co atom. The negative value of θ_P, field induced metamagnetic transition and much lower saturation moment indicate strong antiferromagnetic order at low temperatures. MH curves seem suggest multiple metal magnetic transitions or possibilities of observing magnetization plateau, if one is able to go to 40 to 50 T field. Low temperature neutron diffraction data shows a small additional peak typical of AFM order together with FM like enhancement of intensities of several crystalline peaks, which in turn seem to suggest non-collinear spin structure in this compound.

l0034

Effect of Solvents in Optical Tuning of WS2 Quantum Dots

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Tungsten disulfide (WS_2) is a transition metal di-chalcogenide (TMD) exhibiting luminescent properties when reduced to zero-dimensional size, i.e. quantum dots (QDs). In this work, the solvent effect impacts the optical and structural properties of WS_2 quantum dots (QDs).The QDs have been synthesized in three different solvents using a liquid-phase exfoliation method. The optical properties have been studied using UV-vis absorption and photoluminescence (PL) spectroscopy. The confirmation and size estimation of synthesized WS_2 QDs in various solvents have been done using XRD measurement. The impact of an effective solvent has been observed as an enhancement in optical properties, such as increment in optical band gap and enhanced luminescence effect.The WS_2 QDs in DMSO solvent has the highest band gap as evaluated from UV-Vis absorption spectra and the particle size for the same is smallest. Thus, the UV-Vis study agrees with the XRD study, implying that DMSO is a better solvent for synthesizing WS_2 QDs. DMSO has become an effective solvent that exfoliates the QDs in an efficient manner. The bandgap values estimated from PL emission spectra agreed with the UV-Vis absorption evaluated values. Thus, this research helps understand the role of various solvents in tuning the optical properties of WS_2 QDs.

l0035

Exploring surface reconstruction in Cu2Te: A Scanning Tunneling Microscopic Study

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We explored surface reconstruction in a novel quantum material Cu_2Te by using scanning tunnelling microscope (STM). A surface reconstruction has been observed on the Cu_2Te surface at the atomic level. We observe that the surface reconstruction of UHV-cleaved Cu_2Te involves changes in the arrangement of atoms, which can significantly affect its electronic and physical properties. A distinct and intricate surface reconstruction pattern has been identified even at the large scale area, probably resulting from the interplay between in-plane electron correlations and the interlayer coupling of charge density waves (CDWs) in Cu_2Te. The present results may provide important insights for electronic states of Cu_2Te close to the Fermi level, also it can provide us significant information about some new physical properties of the material.

l0036

Exciton-Phonon Coupling in Two-Dimensional Ruddlesden-Popper Perovskites

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Recently, two-dimensional (2D) metal halide perovskites have garnered significant attention for optoelectronic and spintronic device applications due to their excellent optical and electronic properties. In this study, we conducted a detailed investigation of temperature-dependent photoluminescence (PL) to explore how varying layer numbers affect exciton-phonon scattering in a 2D Ruddlesden-Popper (RP) perovskite, $(TEA)_2(MA)_{n-1}Pb_nI_{3n+1}$ (n=1−3). Our results show that as the layer number (n) increases, both the electron-phonon and exciton-phonon interaction strength are enhanced due to greater lattice mismatch, increased interface complexity and a higher degree of disorders within the system. At low temperatures, the peak of the PL spectrum exhibits a typical red shift for all the layered samples which is primarily due to the combined effects of thermal expansion and electron-phonon interaction. Concurrently, the PL linewidth becomes narrower as the temperature decreases, owing to the suppression of optical phonons. These findings shed light on the underlying causes of various nonradiative processes and scattering phenomena, offering valuable guidance for improving the performance of 2D-RP perovskites in optoelectronic and spintronic devices.

l0037

To Study the Structural, Electronic, and Transport Properties of Armchair GeSeNR - First Principle Approach

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Using the first principle approach, we have probed the structural, electronic, and transport properties of hydrogen-passivated armchair germanium selenide nanoribbons (aGeSeNR) with varying ribbon widths. The negative binding energy value shows the stability of our nanoribbons. Further, we have also calculated the band structure and density of states (DOS) profile, which indicated the semiconducting behavior of our configuration. With increases in the width of aGeSeNRs the stability increases, and also the band gap decreases. In the calculation of transport properties, we made two probe device model with left, and right electrodes and scattering region. We also plot the IV characteristics, which show the simple diode behavior.

t) THESIS PAPERS

t0001

Hydrostatic Pressure Effect on Transport, Magnetic and Superconducting Properties of Non-Centrosymmetric Re_6Hf, $Re_{5.5}Ta$, $(HfNb)_{1.10}(MoReRu)_{0.90}$ and LaPtGe Compounds

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This synopsis consists of seven chapters that describe the introduction of the Non-centrosymmetric (NCS) superconductors. Further, it explored mainly the pressure effect on the transport and magnetic properties of NCS superconductors. The discovery of superconductivity in NCS compounds, which lack inversion symmetry, has encouraged theoretical and experimental investigations because these compounds can host unconventional superconductivity. The NCS systems have received a significant amount of attention over the course of the past decade as a result of their unusual superconducting properties as well as their other fascinating features. The superconducting and normal state characteristics of NCS Re_6Hf, $Re_{5.5}Ta$, $(HfNb)_{0.10}(MoRuRe)_{0.90}$, and LaPtGe have been studied. All of the data from Re-Based -Mn cubic NCS superconductors show a monotonic shift in Tc with P, and the observations of $H_{c2}(0) > H_P$ and $\alpha_M > 1$ at both ambient and high P point to a mixed pairing state as a potential candidate. Moreover, the pressure reported in the tetragonal NCS LaPtGe s-wave superconductor may be an unconventional superconductivity (USC) signature. All research leads us to believe that TRSB may be related to the potential USC signature in non-magnetic NCS superconductors. As a result, it is impossible to rule out the possibility of ASOC in compounds lacking inversion symmetry. To comprehend how the disorder suppresses USC, however, more research in single crystals under high P is required.

t0002

Development of an Uhv-Pld System and Studies on PLD Deposited Y Doped HfO2 Thin Films

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In the present works, an Ultra-High Vacuum (UHV) compatible Pulsed Laser Deposition (PLD) setup was developed at the Angle Resolved Photo Electron Spectroscopy (ARPES) beamline (BL-3) of the Indus-1 synchrotron radiation source (SRS), RRCAT, Indore, India for *in-situ* photoelectron spectroscopic (PES) studies of thin films. The PLD setup allows for quick *in-situ* transfer of deposited films to the analysis chamber, enabling surface-sensitive PES measurements on atomically clean surfaces. Using the developed setup $Hf_{(1-x)}Y_xO_2$ (with x = 0, 0.05, 0.10, 0.15, and 0.20) epitaxial thin films were deposited and investigated for its phase transformation studies using FTIR, XAS, XRD, HRTEM, XPS, and PL techniques. The crystal structure changes from monoclinic to orthorhombic to cubic as the Yttrium (Y) content increases in the HfO_2 thin films. The results indicate that both the doping concentration of Y and oxygen environment are crucial parameters for stabilizing different polymorphs of HfO_2. These findings provide a deeper understanding of phase transitions, local structure, and optical properties, offering pathways to stabilize and identify technologically significant HfO_2 phases for dielectric and ferroelectric applications.

t0003

Quantum Many-Body Phenomena In Charge Density Wave Materials Probed By Light Matter Interactions

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The coupling of electron, phonon, photon, plasmons and spin of an electron provides insights into quantum correlations and existence of multi-body interaction, such as charge density wave (CDW) superconductivity, topological behavior, structural phase transition, and magnetism. CDW is a low temperature strongly correlated ordered phase that arises from periodic modulation of atomic lattice accompanied with the modulations on the electronic charge density. Development of CDW causes superlattice formations, leading to the folding of the Brillouin zone that engenders the emergence of several collective (amplitude and phase modes), two-phonon, and zone folded modes. In this context, the objective of the thesis is to explore, understand and delineate the underlying origins of CDW in layered chalcogenides materials in both bulk and thin flakes. The research aims to elucidate the phonon dynamic of collective excitations and anisotropic light-matter interaction employing Raman spectroscopy as a probing tool, which opens avenues for correlating various aspects of the multi-body phenomenon.

t0004

First-Principles Investigations on Graphene Oxide Derivatives for Photocatalytic Hydrogen Production

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Photocatalytic water splitting for hydrogen generation is an efficient method for the production of clean, sustainable and green hydrogen. Using Van der Waal interaction corrected hybrid density functional theory calculations we have done a comprehensive computational analysis of the structural, thermodynamic, electronic, transport properties, optical absorption, photocatalytic band alignment and photovoltaic properties of graphene oxide derivatives such as graphene monoxide and graphene dioxide. We have adopted several strategies such as varying layer thickness, application of electric field/strain, heterostructure design, isovalent substitutions and isoelectronic co-substitution to tune the properties of these 2D materials. Most of the predicted compositions have direct band gap behavior, optimum optical absorption to harvest the visible part of the solar spectrum, low carrier effective mass values and thus higher mobility resulting enhanced efficiency and several of these materials band edges straddle with the water redox potentials and hence prove to be suitable for visible-light-driven photocatalyst for hydrogen production along with photovoltaic applications.The availability and affordability of the constituents in the proposed compositions will fuel the research on graphene oxide based 2D materials for sustainable energy solutions and accelerate to find efficient path for green hydrogen production and hence motivate experimentalists to make further studies.

t0006

Synthesis, Characterization and Physicochemical Study of Metal and Metal Oxide Based Nanoparticles

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The thesis comprises the synthesis of metal (Ag), metal oxide (ZnO, TiO_2), metal-doped metal oxide (Cr/Cu doped ZnO), ceramic ($BaTiO_3$) nanoparticles (NPs), and Carbon (C quantum dots) using green and/or chemical methods with the physicochemical characterization of prepared samples using different analytical techniques such as XRD, FTIR, Raman, SEM, TEM, EDAX, UV-vis, Photoluminescence, TGA, and zeta potential (ZP) analyzer to study the structural, optical, thermal and ZP properties. Selected samples were γ-irradiated to modify their functionality. A thorough analysis has been carried out using software such as Origin, X'pert Highscore, Fullprof, Vesta, and ImageJ. The samples have been studied for therapeutic and gas-sensing applications. The results have evidenced the high-quality stable NPs with enhanced physicochemical properties that led to better antibacterial, antifungal, antioxidant, hemolytic, and gas sensing applications. The results have been published in high-quality journals and presented at international conferences.

t0008

Engineering Zinc Oxide Electron Transport Layers for MAPbI3 Perovskite Solar Cells

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Electron transport layers (ETLs) in perovskite solar cells (PSCs) are essential in deciding their efficiency, charge collection, and photovoltaic device parameters. Inorganic ETLs like SnO_2, TiO_2, and ZnO are currently employed to fabricate PSCs. Despite its superior optoelectronic properties, ZnO is often overlooked in PSCs due to its chemical instability with metal halide perovskites, requiring modifications like chemical doping and surface passivation. This study focuses on engineering ZnO ETLs by incorporating different concentrations of fullerene (C_{60}) to examine the structural, optical, and device performance of C_{60}-modified ZnO ETLs in $MAPbI_3$ PSCs. The $MAPbI_3$ photoactive layers have been fabricated onto pristine and modified ZnO ETLs using a spin coating technique. Incorporating C_{60} into ZnO reduces microstructural and optical defects, such as micro-strain, Urbach energy, and trap levels, while enhancing the optoelectronic properties of $MAPbI_3$. This leads to better optical properties and improved structural stability, ultimately boosting the performance of photovoltaic devices.

t0009

MXene Reinforced Composites for Thermoelectric Generators with Zero Carbon Emission

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Thermoelectric (TE) materials have great potential to recover waste heat and generate electricity. However, their efficiency has been a major concern for years. Figure of merit (ZT) determines the efficiency of these materials. Till now, various approaches such as doping, nanostructuring, and band engineering have been adopted to enhance their figure of merit. In this work, we have reported the composite formation route using nano inclusions to tailor the thermoelectric performance of TE material. Initially, $Ti_3C_2T_x$ MXene has been synthesized using in-lab prepared Ti_3AlC_2 MAX phase by a cost-effective route. Then, we selectively etched out the Al layer from the MAX phase to get accordion-like MXene sheets. Hereafter, MXene sheets have been incorporated into the earth-abundant and environment-benign thermoelectric materials' matrices such as Bi_2S_3, $SrTi_{0.85}Nb_{0.15}O_3$, and $CoSb_3$ to improve their ZT. Finally, we have observed that MXene has performed exceptionally well with oxide perovskite and showed a maximum ZT of 0.9 above 900 K. We have also demonstrated the highest power output of 38 meV for an n-type 4-leg prototype thermoelectric generator. This study opens new avenues for the synthesis of new generation 2D material MXene for energy applications and proposes an easy & effective approach to improve the efficiency of less-performing thermoelectric materials.

t0011

Studies on Resistive Switching in TiO_2 Thin Films for Non-Volatile Memory Applications

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Resistive Random Access Memory (RRAM) offers a promising alternative to flash memory. TiO_2 is widely studied for RRAM applications, though challenges regarding switching parameters and mechanisms persist. This thesis investigates TiO_2 thin film based RRAM devices with various geometries and electrode materials to improve switching parameters. Reliable unipolar switching was observed in Au/TiO_2/Pt devices with inert electrodes, where faster reset times was achieved at higher reset voltages. Cu/TiO_2/Pt devices fabricated with Cu as active electrode showed bipolar switching with low power and energy consumption and compliance current (I_C) controlled 3-bit multilevel switching. Cu/TiO_2/Pt devices fabricated in 8×8 crossbar geometry exhibited excellent device yield, variability and I_C tunable half-integral quantized conductance states, crucial to achieve high integration density. TiN films fabricated via optimized RF-sputtering, performed similar to Pt, making TiN a viable Pt substitute for RRAM applications. The conducting filament (CF) model explains the switching mechanism, where unipolar switching occurs due to oxygen vacancy-based CF, while bipolar switching is driven by Cu CF-based electrochemical metallization.

t0013

Electrostatic Complexation of Charged Nanoparticle Polyelectrolyte and their Evaporation-Induced Assembly

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The present thesis investigates the intricate phase behavior of multicomponent polyelectrolyte-nanoparticle (penp) systems, driven by the interplay of electrostatic interactions and various entropic forces. Through systematic variation of phase space parameters, we uncover intriguing and tunable phase behaviors in penp complexes, ranging from re-entrant phase transitions to complex coacervation. This tunability presents opportunities to precisely control and manipulate the assembled structures via evaporation-induced assembly (eia). A detailed study of jamming of penp complexes through eia revealed interaction-dependent jamming phenomena within microgranules, highlighting a critical correlation between the phase behavior and jamming characteristics of penp complexes. These silica-amine microgranules has been utilized for co_2 capture and colloidal assembly has shown to have profound effect on the capture capacity which has been further optimized by varying morphological factors.

t0014

A Study of Novel Lead Free Piezoelectric and Magnetoelectric Materials for Multifunctional Applications

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This study investigates novel lead-free piezoelectric and magnetoelectric materials, addressing environmental concerns of lead-based systems. $BaTiO_3$, $BiFeO_3$, and $GdFeO_3$ based compounds were synthesized and characterized for their structural, dielectric, thermal, ferroelectric, piezoelectric, magnetic, magnetoelectric and electrochemical properties. Key findings include improved dielectric, ferroic and magnetoelectric properties in $BiFeO_3$-$GdFeO_3$ composites with enhanced specific heat. A strong magnetoelectric coupling (up to 1.41 $mVcm^{-1}Oe^{-1}$) is observed in Mn doped $BaTiO_3$-$GdFeO_3$ nanocomposites. $BaTiO_3$-$BiFeO_3$ system demonstrated high energy storage efficiency, reaching 72.5%. All the samples exhibit significant values of piezoelectric coefficients(d_{33}). High specific capacitance further highlights their energy storage potential. These lead-free materials show promise for advanced applications in energy storage, magnetic sensors, and data storage devices.

t0015

Defect-induced Tuning of Exchange Bias probed using Au^{8+} Ion Irradiation in Full Heusler Alloy coupled with Antiferromagnet

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We report the impact of swift heavy ion (SHI) irradiation (*i.e.*, 100 MeV Au^{8+}) on the exchange bias field (H_E) and coercivity (H_C) in a series of bottom-pinned $Si/SiO_2/Cu/Ir_8Mn_{92}/Co_2FeAl/Ta$ heterostructure samples grown at room temperature (RT), under the influence of an *in-plane in situ* static magnetic field of 1 kOe. On systematically increasing the Au^{8+} ion fluences from pristine to 3.3×10^{11} ion/cm^2, the positive exchange bias field (PEB) and negative exchange bias field (NEB) experienced enhancements of 30% and 50%, respectively. However, once the ion fluences exceeded the critical threshold of 3.3×10^{11} ion/cm^2 required for creating defects/pinning centers in the antiferromagnetic (AF) layer, a decrease in both H_E and H_C was observed due to interfacial mixing as evident by cross sectional TEM measurements. The augmentation in PEB and NEB is ascribed to the generation of defects or *hyperthermal heating* in the AF layer resulting from ion irradiation. These findings are consistent with the diluted AF model [Miltényi *et al., Phys. Rev. Lett.* **84**, 4224 (2000)].

t0016

Non-Markovian and Non-Gaussian Behaviour in Molecular Diffusion within Complex Fluids

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In this thesis, we advance beyond the traditional Brownian motion model by developing new mathematical frameworks to address non-Gaussian and non-Markovian dynamics. Initially, we studied non-Markovian processes in lipid bilayers using the generalized Langevin equation (GLE). Subsequently, we explored non-Gaussian processes in the cage-jump diffusion of deep eutectic solvents (DESs) through a non-local Fokker-Planck equation. Finally, we combined these aspects by developing the non-Gaussian fractional Brownian motion (nGfBm) model to explain diffusion crossover in glass-forming liquids. Employing quasielastic neutron scattering and molecular dynamics simulations, our work provides robust models applicable across various disciplines, transcending the limitations of traditional Brownian motion theory.

t0018

Carbon Nanotube Based Composite Thin Film Coatings for Stray Light Control Space Applications

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In this work, we discuss emergence of functionalized multi-component structural forms of carbon from single wall carbon nanotubes (SWCNTs) and successful implementation of these low dimensional structural hybrids for stray light control space applications. SWCNTs serve as a building block to give rise to multi structural compounds including multi wall carbon nanotubes (MWCNTs), graphene sheets (GS) and carbon nano scrolls (CNS) after performing oxidative chemical purification and covalent functionalization process. We report a facile, cost effective

and successful fabrication of stable thin film coatings comprised of carbon nano components on the flexible aluminium (Al) substrate that exhibit low reflectance of the order of 2-3% in the visible (Vis) and near-infrared (NIR) spectral band. Fundamental space environmental simulation tests (SEST) performed on the films demonstrate high stability with reflectance values unaltered. We present here our studies on the structure, morphology and optical properties of these films and investigate their performance for low-light scatter applications in adverse space environment.

t0022

Dielectric investigations on Mg salt doped biopolymer electrolytes

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Research studies have shown the possibility of the application of biopolymers in the field of medicine, Wastewater Treatment, Food Packaging Industry etc. For the past 3 decades, the usage of biopolymers for storage devices also proved to be a promising field of study. Tamarind Seed Polysaccharide (TSP) is a best alternative biopolymer electrolyte as compared to synthetic polymers, due to its high biocompatibility, non-toxic nature, excellent mechanical and thermal properties. In the current study, TSP biopolymer is blended with magnesium chloride biopolymer electrolyte films were prepared by solution casting technique. TSP and the dopant salts were taken in the ratios of 90:10, 80:20, 70:30 & 60:40 wt.% for obtaining the films. These films have been subjected to XRD and AC impedance characterization techniques, in order to investigate the structural and dielectric properties. The AC conductivity and dielectric properties of the films were calculated using LCR meter (frequency range: 40Hz – 5MHz). XRD studies revealed that the film TSP:$MgCl_2$ (70:30 wt%) exhibited higher amorphous nature compared to the films of other ratios. As the frequency increased, AC conductivity values increased gradually for the low frequency region and rapidly at the high frequency region. Maximum AC conductivity of the order of 10-5 Scm-1 was observed for the biopolymer film TSP:$MgCl_2$ (70:30 wt%). Dielectric parameters were measured and were found to decrease as the frequency increased. Dielectric constant and the loss values were obtained for the films and they have showed maximum values of 3.87x105 & 2.08x105 for TSP:$MgCl_2$ (70:30 wt%) ratio film. The obtained highest conductivity value for TSP:$MgCl_2$ (70:30 wt%) ratio film was complementary to the results from the XRD analysis.

t0024

Investigation Of Ultrafast Structural Dynamics In Solids Using Time-Resolved X-Ray Diffraction

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The heat dissipation (useful for next-generation device applications) in group IV and group III-V semiconductors/interfaces (InSb, Ge, and GaP/Ge interface) and nonlocal probing of amplitude dynamics (AM) in novel $EuTe_4$ in its charge density wave (CDW) phase are studied using the time-resolved X-ray diffraction (TXRD, an optical pump X-ray probe) technique. The TXRD setup is developed using laser plasma Cu K_α X-ray source (probe). The K_α is generated by the interaction of ~50 fs, 1 kHz Ti:sapphire laser pulses with Cu wire target, which is synchronized with the pump pulse. A Laue diffraction pattern from the $EuTe_4$ crystal is recorded for the first time using this source. The heat dissipation (thermal strain propagation) study indicates recovery at ~1.5 ns in InSb (111) sample and trapping of heat in GaP epilayer in GaP/Ge hetero-structure. A long-lasting deformation potential effect (~100 ps) in Ge (111) after photo-excitation is observed (earlier reported for <1ps). The nonlocal behavior of the AM is from propagating phonon-polariton, observed for the first time in any CDW compound due to the polar nature of the AM in $EuTe_4$ and provides an opportunity to engineer material properties at fs time scale with optical pulses.

t0025

Crystal structure and electrical properties of lead-free ferroelectric materials

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Ferroelectric and piezoelectric materials are crucial for modern technology, including electronics, communication, healthcare, and energy storage. The use of lead-based materials poses significant environmental risks due to lead toxicity, prompting research into lead-free alternatives. We synthesized and studied the structural and electrical properties of x $Na_{0.5}Bi_{0.5}TiO_3$ (NBT)-(1-x)($NaNbO_3$(NN)/$BaTiO_3$(BT)) materials. Our study identified a direct transition from the room temperature ferroelectric (FE) rhombohedral (R3c) to the paraelectric (PE) cubic (P) phase at elevated temperature in xNBT-(1-x)NN/BT (x=0.95, NBT-NN05/BT05) which bypassed the intermediate tetragonal phase, influenced by variations in lattice strain due to A-site (Ba) modifications. Furthermore, we found Na^+ ions significantly contributed to electrical conductivity at high temperatures in NBT-NN05. A phase diagram for xNBT-(1-x)NN showed coexistence of orthorhombic, tetragonal, and rhombohedral phases over different compositions. The phase transitions indicated a first-order nature, corroborated by dielectric and Raman scattering studies. Additionally, a temperature-dependent structural study on 0.05NBT-0.95NN(05NBT) demonstrated relaxor behavior without structural transitions below 300K, and four phase transitions above room temperature. These transitions were supported by dielectric anomalies and Raman spectral changes, revealing local structural changes. This work advances the understanding of NBT-based lead-free ferroelectrics for developing advanced materials and technologies.

t0031

Superalkali OLi_3 Anchored Biphenylene for Hydrogen Storage: Acumen from First-Principles Study

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Developing effective methods and materials for storing hydrogen is essential for shifting our dependency on the traditional fossil fuels in the transportation sector. In this regard, using the first-principles study in the domain of density functional theory, we have examined the storage potential of the superalkali OLi_3-anchored biphenylene sheet. OLi_3 cluster binds to BPN sheet due to charge transfer mechanism. With both-side coverage, the OLi_3 cluster exhibits a strong binding affinity with BPN, -3.05 eV/OLi_3 binding energy. 2OLi_3/BPN complex can adsorb 18 H_2 molecules due to electrostatic and van der Waals interactions and the adsorption energy ranging from -0.217 to -0.282 eV, achieving an H_2 gravimetric density of 9.11 wt%, exceeding the standard hydrogen storage requirement set by the Department of Energy, 5.5 wt%. Using van't Hoff equation, the calculated desorption temperature of 2OLi_3/BPN+18H_2 complex is 258 K at 1 atm and 337 K at 5 atm. Ab-initio molecular dynamics simulations validate the structural stability and the H_2 reversible behavior. With the appropriate H_2 adsorption energy, high gravimetric density, and structural stability, it is expected that the use of OLi_3-anchored BPN sheets will serve as an effective method with high-capacity reversible hydrogen storage.

y) YOUNG ACHIEVER PAPERS

y0001

Augmented Electrochemical Performance in Composite Electrode Material for Supercapacitor Application

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Conducting polymers, including, PIn, PANI and PPy, were integrated with rare earth metal oxides (Nd_2O_3, Yb_2O_3, Eu_2O_3, Gd_2O_3), carbon nano-onions (CNOs), carbon black (CB), and MoS_2 sheets to enhance their charge storage capabilities. Electrochemical characterization revealed that the composites exhibited improved specific capacitance and cycling stability compared to pure polymers. Specifically, PANI composites demonstrated notable enhancements in capacitance retention after 100 cycles, reaching up to 84.92% with Nd_2O_3 and 80.55% with CNOs. PPy composites, incorporating Yb_2O_3 and Eu_2O_3, showed initial coulombic efficiencies above 80% and stable cycling performance at high rates. Moreover, MoS_2-incorporated ternary composites (PIn/CB/MoS_2) exhibited superior capacitance due to enhanced surface area and improved ion accessibility. These findings highlight the effectiveness of modifying polymer matrices with inorganic fillers to achieve enhanced electrochemical performance, making them promising candidates for advanced supercapacitor technologies.

y0003

Vibrating Sample Magnetization (VSM) And Structural Characterization of Ferrite and Ferroelectric ($Batio_3$) Composites

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The material possessing piezoelectric and magnetostriction effect i.e magnetoelectric composites with general formula $(1\text{-}x)Ni_{0.5}Cu_{0.3}Mg_{0.2}Fe_2O_4 + (x)BaTiO_3$ in which x = 0, 0.20, 0.40, 0.60, 0.80 and 1 mol were prepared by conventional solid state reaction. The presence of constituent phases in the composites was confirmed by x-ray diffraction studies. The hysteresis behavior studied to understand the magnetic properties such as saturation magnetization, Remanent magnetization, Coercive field, and magnetic moment. The magnetic properties of above mentioned sample were investigated by using Vibrating Sample Magnetometer (VSM) at room temperature. The presence of ferroelectric phase affects the values of Saturaton magnetization (Ms), Coercivity (Hc), and Remanent magnetization (Mr). The values of saturation magnetization and remanent magnetization decreases as the content of magnetic material i.e. ferrite decreases and the values of coercive field and remanence ratio increases as ferrite content decreases. The coercivity of the composites increases with $BaTiO_3$ addition.

y0004

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.

y0005

Structural and Transport Studies of Tellurium Single Crystal Grown by Open-Ended Chemical Vapor Transport

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Here, we report the open-ended chemical vapor transport (CVT) growth method and the structural and transport behavior of successfully grown tellurium (Te) single crystal. Te crystals from micrometers to millimeters in size can be grown with this fast method. Te single crystals are grown in direction [1 0 0] and elongated in direction [0 0 l]. Trigonal single phase and the space group $P3_121$ of grown Te single crystals are confirmed by Rietveld refinement of powder X-ray diffraction (XRD). The positive value of microstrain in crystal suggests the local compressive strain due to dislocations and grain boundaries. The rocking curve of (100) peak in high-resolution X-ray diffraction (HRXRD) confirms the presence of low-angle grain boundaries and other lattice defects. The crystal with electron concentration $n \sim 6.4\times10^{15}$ cm^{-3} shows an upturn at low temperature in resistivity and the logarithmic temperature dependence of resistivity suggests a one-dimensional variable range hopping (VRH) mechanism.

y0006

Role of Non-Magnetic Scandium in Elucidating the Cluster Spin Glass Behavior of $Pb(Fe_{0.5}Nb_{0.5})O_3$

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Abstract We report the role of non-magnetic scandium (Sc) to uncover the nature of spin glass behavior of $Pb(Fe_{0.5}Nb_{0.5})O_3$. Sc substituted compounds $Pb(Fe_{0.5-x}Sc_xNb_{0.5})O_3$ ($0 \le x \le 0.15$) were synthesized via wolframite precursor method. X-ray analysis confirm the synthesized compounds were stabilized in monoclinic crystal symmetry. The anomalies found in field-cooled (FC) and zero field-cooled (ZFC) magnetization curves indicates the anti-ferromagnetic and spin glass features. The characteristic irreversible temperature (T_{irr}) decreases with increasing magnetic field across all the compounds studied. Broad ZFC peak and a plateau region found in FC curve over small temperature range demonstrate the ground state cluster spin glass character of these compounds. The spin-glass freezing temperature of the compounds was determined using Almeida –Thouless (AT) line and analyzed. Raise in the spin-glass freezing temperature (T_f) at lower Sc content attributed to the enhanced cluster size driven by B-site cation ordering. The results suggest that the impact of Sc substitution on the magnetic properties of $Pb(Fe_{0.5}Nb_{0.5})O_3$ caused a change spin-glass freezing temperature and manifest the cluster spin glass ordering of the $Pb(Fe_{0.5-x}Sc_xNb_{0.5})O_3$ compounds.

y0007

Development of Al assisted Versatile Chemical Sensor Arrays for On-demand End Use

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Gas sensors are the semiconductor devices that are capable of detecting gaseous components from the atmosphere via surface state interactions of semiconductor materials. So far, the field has matured to make its mark in technology but is limited by materials that sense at room temperature and are specific. From the device perspective it leads to high power consumption and lacks selectivity. Besides sampling gases in real-time condition often involves a mixture of gases rather than just one test gas in the background air or nitrogen. Thus, we have developed a range of sensor arrays that are a mix of semi-selective and non-selective sensors to sample out volatile organic compounds (VOCs) in a mixture. We device strategies to train AI algorithms in different fashions and seek robust predictions as a result of feature engineering. These VOC sensors find wide-spread utility in process control, diagnostics, breath analysis etc.

y0008

Energy Harvesting by Cellulose-PEDOT: PSS Aerogel-Based Triboelectric Nanogenerator

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TENG has emerged as a promising nanotechnology for sustainable energy harvesting based on the coupling effect of triboelectrification and electrostatic induction. In this work, we have simulated a TENG device by COMSOL Multiphysics to obtain the electric potential distribution across different separation distances of tribopostive, and tribonegative layers. Based on the simulated model, we have fabricated a cellulose-PEDOT: PSS aerogel and PDMS-based TENG and analyzed its potential for health monitoring applications. The synthesized material is characterized

using FTIR, and SEM and their electrical output is measured by operating the TENG in contact separation mode. The efficient output of the device (Voc up to 60 V, Isc up to 100 nA, and Qsc up to 50 nC) can power smaller electronic circuits like LEDs and can charge capacitors. The performed study promises effective applicability in mechanical energy harvesting and further possibilities in health monitoring devices.

y0011

Electronic, Elastic and Thermoelectric Investigation on CoHfAs Heusler Alloy

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In this work, the Quantum Espresso package is utilized within the framework of Kohn Sham density function formalism with the Perdew-Burke-Ernzerh generalized gradient approximation to calculate the structural, electronic, and elastic properties of half-Heusler alloy CoHfAs. Using ultra-soft pseudo-potential, structural optimizations are carried out at different atomic positions to calculate the ground state properties, such as the lattice parameter and bulk modulus. The electronic properties of the alloy around the Fermi level, for both spin-up and spin-down bands, are calculated, and it shows a semiconducting behaviour with an indirect band gap of 1.24 eV. Elastic properties (C_{11}, C_{12}, and C_{44}) are calculated to satisfy the Born-Huang stability criteria of the material. The obtained positive phonon frequencies also suggest the material's stability. Temperature-dependent thermoelectric properties such as the Seebeck coefficient, electrical conductivity, and thermal conductivity are calculated in the temperature range of 100–1000 K. Hence, the power factor and the dimensionless figure-of-merit (zT) are estimated. Our calculated results show that the CoHfAs alloy is a potential candidate for high-temperature power generation.

y0016

Anisotropic Superconductivity in Bismuth Single Crystals

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At ambient pressure, bismuth (Bi) crystalizes in a rhombohedral crystal structure and is a semimetal. Theoretically a superconducting ground state in bulk Bi at ambient pressure was ruled out owing to extremely low charge carrier density ($n = p \sim 3 \times 10^{17} cm^{-3}$), but our recent experiments have demonstrated bulk superconductivity in ultrapure (99.9999%) Bi single crystals below 0.53 mK, with an estimated critical magnetic field $H_C = 5.2\ \mu T$ at 0 K[1]. Here, we report the temperature dependence of the upper critical field along different crystallographic directions. The critical field measurements along $H||[0001]$ (trigonal) axis and $H||[01\bar{1}0]$ (bisectrix) crystallographic axis show that the upper critical field in Bi is anisotropic with an anisotropy ratio of $H^{[0001]}(0)/H^{[01\bar{1}0]}(0) = 3.1$. These findings suggest that the conventional Bardeen-Cooper-Schrieffer (BCS) cannot account for the superconductivity in Bi and suggests that we need a mechanism beyond conventional electron-phonon coupling to explain superconductivity in Bi.

y0018

DFT Based Theoretical Investigation of Transition Metal Effect in Molybdate Alluaudite

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There has always been an interest in studying the electrocatalytic performance of battery materials. In this work, a polyanionic compound molybdate alluaudite which is well known cathode material used in sodium ion battery, has been explored for electrocatalytic performance. Two different molybdate alluaudites are investigated for oxygen evolution (OER) and oxygen reduction reaction (ORR) by changing the *3d* transition metal (TM) element components. The theoretical investigation to probe OER and ORR, is primarily based on interaction of reaction intermediates with the *Ni*- and *Co*-molybdate alluaudite as obtained from the first principles calculations under the framework of density functional theory (DFT). The systematic electronic structure calculations actually help to explain how the local electronic structure and interaction of reaction intermediates with the catalyst surface influence the OER and ORR activity once we move from Ni based molybdate to Co based molybdate alluaudite.

y0019

Imprinting scalar spin chirality by anisotropic strain in a Kagome antiferromagnet

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Application of strain in epitaxial thin films has been a productive strategy to control material properties, promising realization of "materials by design". Here, we extend the concept to topological Kagome antiferromagnets, which can host a variety of exotic magnetic states. One such compound, Mn_3Sn, has an inverse triangular spin order that is non-collinear but coplanar and hence, does not possess scalar spin chirality. We show anisotropic strain in addition to Dzyaloshinskii-Moriya interaction in heterostructures of epitaxial Mn_3Sn thin films can stabilize a magnetic ground state with manganese spins canting out of the Kagome plane with a finite scalar spin chirality that induces a large Berry phase in the momentum space. This results in the emergence of anomalous Hall e↵ect in the Kagome plane at room temperature, which can be fully switched by charge current while allowing access to multiple resistance states depending on the bias field.

y0020

Symmetry-Breaking Interactions and Magnetic Frustration Induced Topologically Protected Spin Textures in Layered Magnets

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Topologically protected magnetic spin textures are known to emerge via electron spin in various magnetic materials. These solitonic structures can be driven by low current density or electric fields, bearing potential to be stabilized in nanoscale dimensions, offering new directions for development of spintronics-based future quantum devices. However, there remain some fundamental roadblocks pertaining to the difficulty to realize ultrasmall stable skyrmions with tailored sizes and clarification of the underlying fundamental interactions necessary for the stabilization of unconventional spin textures in various magnetic systems. Here, we demonstrate two novel phenomena: (a) interplay of interfacial Dzyaloshinskii-Moriya interactions (DMI) and magnetic frustration at reduced dimensions, and (b) bulk antisymmetric DMI, and experimentally demonstrate their capabilities for stabilization of a plethora of spin structures in layered magnetic systems. Our results offer a promising pathway towards realization of various spin-textures with tailored properties for spintronic and quantum device applications.

y0021

Manipulating Flow of Light in Multilayer Thin Films for Optical Coating Devices

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Understanding and mastering the intricacies of manipulating the flow of light in multilayer thin films is essential for developing optical coating devices for applications in making of optical and scientific instruments, lasers, telecommunications, smart windows, sensors, imaging, display and lighting, etc. Fundamental principle of thin film optics including interference, dispersion, plasmons, and polarization have been explored in dielectric/dielectric and metal/dielectric multilayer thin films for tailoring reflection, transmission, and absorption of a medium, enabling

precise control and modulation of light. The synergistic interplay between thin film layers composed of two different materials allows making the optical coating devices with unprecedented functionalities. This article discusses overview of our research on optimization of optical properties and morphology of single layer films, material combinations, multilayer design strategies, and deposition techniques vital for the realization of such multilayer coatings. Finally, it presents the development of a few customized multilayer coatings such as wideband antireflection coating, omnidirectional high reflectivity mirror, non-polarizing beam splitters, and UV bandpass filters required for different departmental projects.

y0023
Spin-Orbit Coupled Oxide Heterostructures: At the Intersection of Topology and Antiferromagnetic Spintronics
Megha Vagadia
Abstract: TBA

y0024
Two Tales of Fractionalisation in Quantum Spin Systems
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Fractionalization in quantum spin liquids (QSLs) is one of the outstanding quests of modern condensed matter physics. In this manuscript we present our recent works on two different aspects of fractionalisation in quantum spin systems. First: Low-energy physics physics of quantum spin liquids contains unusual degrees of freedom, such as emergent gauge fields and fractionalized excitations, projective symmetry group (PSG) approach allows one to systematically classify all such possible fractionalised excitations that are consistent with the symmetry of the system. In this work we develop various practical ways to employ PSG approach for frustrated magnets. Specifically, we present our results of an extensive study of a mean field theory of possible fermionic fractional excitations in a U(1) QSL on dipolar octupolar magnets. Several of these mean-field states show a linear temperature dependence of specific heat at low temperatures, the other phases show a power law temperature dependence of specific heat. The linear temperature dependence of specific heat at low temperatures is reminiscent of the observations in Nd_2ScNbO_7. Second: Fractons are excitations in a many body system which can be mobile only as a pair in a fractional subspace of the the full system. The realization of these aberrant mobility constraints and subsystem symmetry in physical systems is not naturally available. In this work we overcome this limitation and propose an essentially exact physical realization of fractonic quasiparticles with subsystem dipolar symmetry in a 2D non-degenerate, ordered spin system with local two-spin interactions.

y0025
Magnetic field tunable ground states in frustrated low-dimensional antiferromagnets: materials design and emergent phenomena
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Abstract. The emergent quantum critical phenomena's from the lattice are originates from the interplay of lattice, orbital, charge, and spin degrees of freedom, resulting in various ordered patterns/states. The properties of such material classes result from competitions among several factors: crystal electric field splitting (CEF), Coulomb repulsion, Hund's rule, and spin-orbit coupling (SOC). The low dimensional frustrated quantum magnets with different lattice topology, for instance 2D planner, 1D zigzag chain and tunnel geometry lattices are an active field of research in current condensed matter physics and are of my research interest since recent few years and discovered several new to 3*d* as well as 4*d* transition metal based quantum materials and explore their ground state properties and modest SOC physics [Ref. 1-5]. In addition to their intrinsic features related to frustrated lattice, these systems exhibit diverse and unusual novel quantum phenomena under external magnetic field. In our recent work we report a comprehensive investigation of the highly intertwined novel examples of such new low-dimensional 3*d* and 4*d* transition metal based systems [Ref. 1-5]. This includes materials design of several new quantum magnets such as $Ba_2(Co,Ni,Mn)(PO_4)_2$, $NaRu_4O_9$, $Na_{2.7}Ru_4O_9$, $(Cu,Ni)_2V_2O_7$ and $CaCoV_2O_7$ followed by exploring their emergent phenomena. However, in my Young Achiever Award (YAA) talk at 68th DAESSP, I will briefly describe various new discovered condensed matter phases by me, but most of my talk will particularly focus on our recent discovery of novel sharp quantum phase transition as found in new condensed matter system with Co^{2+} as a magnetic Kramer's

active ions which are forming zigzag frustrated chains in $CaCoV_2O_7$ [Ref. 1], induced by an applied magnetic field. Further, below T_N = 3.3 K our zero-field neutron diffraction studies reveled the ↑↑↓↓ antiferromagnetic ground sate spin structure, which is stabilized by an order-by-disorder phenomenon. At base temperature, the magnetic order is suppressed by an applied magnetic field (B), inducing a transition into a quantum paramagnetic state at B_c = 3 T, as revealed by both neutron diffraction and ESR results. The transition exhibits an unusually sharp phase boundary with the critical exponent as found to be $\phi = 0.164(3) \approx 1/6$, is in sharp contrast to the earlier experimental observations for a uniform spin-1/2 chain systems. Such a sharp QPT is anticipated due to a rare combination of SOC and competing NN and NNN exchange interactions J_1 and J_2 of the zigzag spin chain.