# 69th DAE Solid State Physics Symposium

## December 19-23, 2025

# Abstract Book

*Organized by*

***Bhabha Atomic Research Centre***
***Mumbai, India***

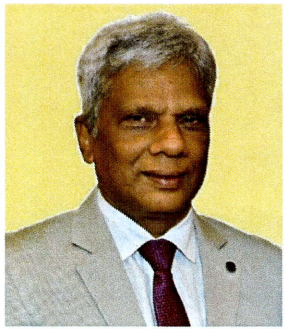
*Sponsored by*

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

*Venue*

***Indian Institute of Technology Roorkee,***
***Uttarakhand - 247667***

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

I am happy to note that the 69th DAE Solid State Physics symposium is being organised by Bhabha Atomic Research Centre at the Indian Institute of Technology, Roorkee, Uttarakhand, India during December 19-23, 2025. This symposium over the years has kept its high scientific standard as well as has maintained its popularity in the condensed matter physics community of the country, particularly among the PhD students and young researchers. The interest can be judged by submission of a large number of papers in this symposium by researchers from across the various institutes and universities of the country, among which 680 papers selected by peer reviewing will be presented in the symposium in the form of poster and oral presentations.

The platform provided by this symposium is used not only to present the latest experimental and theoretical scientific findings but also to facilitate scientific interactions and foster discussions between young researchers and eminent senior scientists and it is also nice to see that this year over 40 eminent scientists from India and abroad will attend this symposium to deliver plenary talks, special evening lectures and invited talks.

I send my best wishes to all the delegates of this symposium for fruitful scientific interactions over this five day event and a grand success to the symposium.

Ajit Kumar Mohanty

(Ajit Kumar Mohanty)

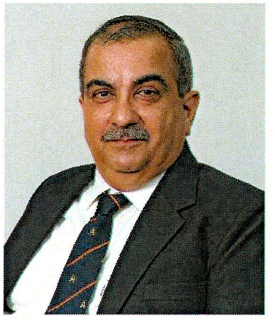
राष्ट्र की सेवा में परमाणु
प ऊ वि
DAE
ATOMS IN THE SERVICE OF THE NATION

अणुशक्तिभवन, छत्रपति शिवाजी महाराज मार्ग, मुंबई - 400 001, भारत • Anushakti Bhavan, Chhatrapati Shivaji Maharaj Marg, Mumbai - 400 001, India
दूरभाष/Phone:+(91) (22) 2202 2543 • फैक्स/Fax: +(91) (22) 2204 8476 / 2284 3888
ई-मेल/E-mail: chairman@dae.gov.in

विवेक भसीन
**Vivek Bhasin**

भारत सरकार
**Government of India**

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



# MESSAGE

It gives me great pleasure to note that the DAE Solid State Physics Symposium (DAE SSPS) has entered into the glorious 69th year of successful organisation. DAE SSPS is among the oldest scientific events of the country and among the most prestigious in the field of condensed matter physics. Particularly, PhD students and young researchers look forward to attend this symposium every year to present their latest theoretical and experimental results in this field. The symposium is organised by Bhabha Atomic Research Centre every year in different parts of the country and this year it is being held at the Indian Institute of Technology Roorkee, Uttarakhand, India during December 19-23, 2025.

I am happy to see that more than 680 papers will be presented in this symposium by researchers from various DAE institutes, Universities and other premier institutions of the country and will cover a broad range of topics including phase transitions under high pressure and temperature, physics of soft matter including biological systems, nano-materials, novel experimental techniques and devices, physics of surfaces, interfaces and thin films, computational condensed matter physic, physics of functional materials including ferroelectrics, piezoelectrics, semiconductors and topological insulators, spintronic materials, materials for energy and environmental applications and quantum materials. The best thesis and young achiever categories have also received significant response showing the popularity of these events among the young scientific community of the country. It is also nice to see that over 40 eminent scientists from India and abroad will deliver plenary, special evening lectures and invited talks in this symposium and will interact with the young researchers over the five-day event.

I wish a grand success to this event and fruitful scientific deliberations among young researchers and eminent scientists during the symposium.

(Vivek Bhasin)

27.11.2025

भाभा परमाणु अनुसंधान केंद्र, ट्रॉम्बे, मुंबई- 400 085, भारत • Bhabha Atomic Research Centre, Trombay, Mumbai 400 085, India
दूरभाष/Phone:+(91) (22) 2550 5300, 2551 1910 • फैक्स/Fax: +(91) (22) 2559 2107, 2550 5151
ई-मेल/E-mail: director@barc.gov.in

भारतीय प्रौद्योगिकी संस्थान रुड़की
रुड़की – 247667(उत्तराखण्ड), भारत

**INDIAN INSTITUTE OF TECHNOLOGY ROORKEE**
Roorkee - 247 667 (Uttarakhand), India

T: +91 - 1332–272742, 285500 (O), 9837070794 (O)
F:+91 - 1332 –285815, 273560
E: director@iitr.ac.in,dir_office@iitr.ac.in

प्रो० के० के० पंत
निदेशक

**Prof. K.K. Pant**
Director

**Message**

It is with great pleasure that I extend a warm welcome to all delegates, participants, distinguished guests, and invitees attending the 69th DAE Solid State Physics Symposium (DAE-SSPS 2025), hosted by the Indian Institute of Technology Roorkee from December 19 to 23, 2025.

The Department of Physics at IIT Roorkee is truly honored to host this prestigious event, organized under the auspices of the Bhabha Atomic Research Centre (BARC) and the Department of Atomic Energy (DAE). This symposium serves as a testament to the ongoing commitment to excellence in solid state physics, bringing together leading scientists, researchers, early-career scholars, and students from across India and beyond. It provides a platform to share groundbreaking advancements in condensed matter science, materials research, and related fields that are crucial for our nation's scientific and technological advancement.

At IIT Roorkee, we are proud to foster an environment that encourages intellectual exchange on diverse topics in condensed matter physics, including quantum materials, nanomaterials, spintronics, topological phases, and emerging technologies in energy and electronics. These areas not only align with our institute's legacy of innovative research and education but also contribute to solving real-world challenges in sustainable development and high-tech industries. IIT Roorkee has a long-standing tradition of close collaboration with BARC as well as DAE institutions, with our researchers extensively using national facilities for neutron, x-ray, high magnetic field, and pulsed-current sources to carry out cutting-edge experiments in condensed matter physics.

We are deeply grateful to BARC and DAE for their steadfast support and for entrusting IIT Roorkee with the responsibility of hosting this landmark symposium. This partnership exemplifies the collaborative spirit that strengthens the condensed matter physics community in India, fostering deeper connections among our faculty members and the esteemed participants.

We are confident that this symposium will serve as a fertile ground for intellectual exchange, sparking new ideas, forging innovative partnerships, and making meaningful contributions to the field. On behalf of the entire IIT Roorkee community, I wish you a productive, inspiring, and memorable experience that will leave a lasting impact.

(K K Pant)

Dr. T. Sakuntala
Director, Physics Group
निदेशक, भौतिकी वर्ग,
Tel.: +91-22-25593883
Email: sakuntl@barc.gov.in

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

It gives me immense pleasure to greet the organizers and welcome all the participants of 69th Symposium organized by the Department of Atomic Energy. Popularly known as the DAE-Solid State Physics Symposium, SSPS is a flagship national symposium organized by the Physics Group of Bhabha Atomic Research Centre. This symposium holds a special place for the solid-state research community of India, especially young students and researchers. With a view of recognizing and nurturing talented scientists, it has been a practice to hold this symposium in different part of the country. This year it is organized at IIT-Roorkee, which has a very rich history as a premier institute for engineering & technology.

I am very much hopeful that, as in the past, the 69th DAE SSPS 2025 would give a scientifically enriching experience to all the participants, serve to motivate several new discoveries, and also bring about networking among research groups. I would like to thank and acknowledge the team at IIT Roorkee and my colleagues from Physics Group of BARC, who have worked hard to bring out an excellent scientific program along with all the hospitality arrangements for the participants. I also take this opportunity to thank the Director IIT-Roorkee and Director, BARC for their encouragement and strong support. My best wishes for the grand success of DAE-SSPS 2025.

Sakuntala

(T. Sakuntala)

भारत सरकार
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भाभा परमाणु अनुसंधान केन्द्र
**BHABHA ATOMIC RESEARCH CENTRE**
अनुप्रयुक्त वर्णक्रमदर्शिकि प्रभाग
**ATOMIC & MOLECULAR PHYSICS DIVISION**

ट्रॉम्बे
मुंबई 400 085
TROMBAY
MUMBAI 400085

Dr. D. Bhattacharyya
Outstanding Scientist &
Head, Atomic & Molecular Physics Division
Bhabha Atomic Research Centre
Mumbai – 400 085, INDIA
& Professor, Homi Bhabha National Institute
Anushaktinagar, Mumbai – 400 094, INDIA
Editor, Journal of Synchrotron Radiation (IUCr)

## Message

This is the 69th glorious year of the Department of Atomic Energy - Solid State Physics Symposium (DAE SSPS), one of the most prestigious scientific conferences in the field of condensed matter physics and this year it is being held at the Indian Institute of Technology Roorkee, Uttarakhand, India during December 19-23, 2025. It is a matter of great privilege and also of big responsibility to serve as a convener of the 69th DAE SSPS 2025.

This year, we had received nearly 800 manuscripts from various DAE institutes, Universities and other premier institutions across the length and breadth of the country under the 11 categories covering almost all important topics of current importance viz., phase transitions under high pressure and temperature, physics of soft matter including biological systems, nano-materials, physics of surfaces, interfaces and thin films, computational condensed matter physic, physics of functional materials including ferroelectrics, piezoelectrics, semiconductors and topological insulators, spintronic materials, materials for energy and environmental applications and quantum materials. Nearly 33 coordinators and around 431 reviewers from across the country helped us to review these manuscripts and finally around 680 manuscripts have been selected for presentation in this symposium. The best thesis and young achiever categories have also received significant response manifesting the impact of these events among the young scientific community of the country. Over 40 eminent scientists from India and abroad have accepted our invitation to deliver plenary, special evening lectures and invited talks in this symposium. We urge all young researchers and PhD students to use this opportunity to interact with the experts to scientifically enlighten themselves further and to initiate possible collaborations.

I would like to acknowledge the efforts of Dr. Himal Bhatt and Dr. Niranjan S. Ramgir, the scientific secretaries of the symposium who have worked very hard to chalk out the well-planned scientific program spreaded over the 5 days. I sincerely thank the local convener Prof. V.K. Malik of IIT Roorkee and his colleagues for their tireless effort in making all the arrangements for hosting the symposium successfully and making the stay of the delegates comfortable.

I look forward to see the 69th DAE SSPS 2025 a great success with enriching scientific deliberations and fruitful interactions among the delegates during the symposium.

Yours sincerely,

Date: 09th December, 2025

(D. Bhattacharyya)
Convener, 69th DAE SSPS 2025

# Patrons

| Name | Affiliation |
|---|---|
| A.K. Mohanty | DAE, Mumbai |
| Vivek Bhasin | BARC, Mumbai |

# Advisory Committee

| Name | Affiliation |
|---|---|
| T. Sakuntala | BARC, Mumbai |
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| M. Krishnamurthy | TIFR Hyderabad, Hyderabad |
| U. Kamachi Mudali | HBNI, Mumbai |
| A.K. Tyagi | HBNI, Mumbai |
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| S. Ramakrishnan | IISER, Pune |
| A. Sundaresan | JNCSR, Bengaluru |
| G. Ravikumar | GITAM, Vishakhapatnam |

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| D. Bhattacharyya (Convener) | BARC, Mumbai |
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| V. K. Aswal | BARC, Mumbai |
| V. Sathe | UGC-DAE-CSR, Indore |

## SUBJECT CATEGORIES

**a)** Phase transitions and dynamics

**b)** Soft matter including biological systems

**c)** Nano-materials

**d)** Experimental techniques and devices

**e)** Surfaces, interfaces and thin films

**f)** Computational, AI and ML methods in condensed matter physics

**g)** Dielectric, ferroelectric and piezoelectricmaterials

**h)** Transport properties and semiconductorphysics

**i)** Magnetism and superconductivity

**j)** Energy and environmental materials

**k)** 1-D, 2-D and quantum materials

## AWARD CATEGORIES

**t)** Thesis

**YAA)** Young Achiever Award

# Programme Overview

<table>
<tr><th colspan="3">Day 1: Friday, December 19, 2025</th></tr>
<tr><td>08:00-09.30</td><td colspan="2">Registration<br>(Venue: Reception area Convocation Hall)</td></tr>
<tr><td>09.30-10:30</td><td colspan="2">Inaugural Function (Venue: Convocation Hall)</td></tr>
<tr><td>10:30-11.15</td><td colspan="2">Technical Session-1<br>Plenary Talk-01<br>Olof Karis (MAX IV, Sweden)<br>MAX IV Laboratory – Prospects For Advancing Synchrotron Science Into The 2030s</td></tr>
<tr><td>11:15-12:15</td><td colspan="2">High Tea & Group Photo</td></tr>
<tr><td>12:15-13:00</td><td colspan="2">Technical Session-1 (Contd…)<br>Plenary Talk-02<br>Sakura Pascarelli (European XFEL, Germany)<br>New scientific opportunities at the European X-ray Free Electron Laser</td></tr>
<tr><td>13:00-14:00</td><td colspan="2">Lunch Break</td></tr>
<tr><td rowspan="4">14:00-15:30</td><td>APJ-AKB Lecture Hall 1</td><td>APJ-AKB Lecture Hall 2</td></tr>
<tr><td>Technical Session-2<br>(Infra-red/Terahertz Spectroscopy in Probing Condensed Matter)</td><td>Technical Session-3<br>(Theoretical Condensed Matter Physics)</td></tr>
<tr><td>Invited talk –1<br>Ewald Janssens, KU Leuven, Belgium<br>Tunable mid-infrared plasmonic metasurfaces<br>Invited talk –2<br>S. S. Prabhu, TIFR, Mumbai<br>Far-Field, Near-Field and Time Resolved Terahertz (THz) Spectroscopy of Materials</td><td>Invited talk–4<br>G. P. Das, RISE, TCG-CREST, Kolkata<br>The emerging world of topological semimetals<br>Invited talk –5<br>S. Balasubramanian JNCASR, Bangalore<br>Boroxol Ring Fraction in $B_2O_3$ Glass (theory)</td></tr>
<tr><td>Invited talk-3<br>M.K. Chattopadhyay, RRCAT, Indore<br>A facility for studying condensed matter using the intense MIR radiation from an FEL</td><td>Invited talk-6<br>Narayan Mohanta, IIT Roorkee<br>Quantum phenomena in planar Josephson junctions</td></tr>
<tr><td>15:30-16:00</td><td>Contributory Oral presentations<br>e0025, k0006<br>(2 nos.)</td><td>Contributory Oral presentations<br>f0014, d0001<br>(2 nos.)</td></tr>
<tr><td>16:00 - 18:00</td><td colspan="2">Tea + Poster Presentation: Contributory paper + YAA (20)</td></tr>
<tr><td>18:30 - 19:00</td><td colspan="2">Evening talk –1 (Convocation Hall)<br>Sanjay K Rai, RRCAT, Indore<br>Research using Indus and possibilities with 4th generation High brightness Synchrotron Radiation source</td></tr>
<tr><td>20:00</td><td colspan="2">Dinner</td></tr>
<tr><th colspan="3">Day 2: Saturday, December 20, 2025</th></tr>
<tr><td rowspan="2">09:30-10:15<br>10:15-11:00</td><td colspan="2">Technical Session-4<br>Plenary talk –03<br>Kalobaran Maity, IACS, Kolkata<br>Dirac Fermions in The Presence of Electron Correlation</td></tr>
<tr><td colspan="2">Plenary talk –04<br>Cristian Bernhard, University of Fribourg, Switzerland<br>Magnetic, orbital, ferroelectric, and superconducting orders in $YBa_2Cu_3O_7/Nd_{1-x}(Sr,Ca)_xMnO_3$ multilayers</td></tr>
<tr><td>11.00-11.30</td><td colspan="2">Tea Break</td></tr>
</table>

| 11:30-12:30 | APJ-AKB Lecture Hall 1 | APJ-AKB Lecture Hall 2 |
|---|---|---|
| | **Technical Session-5**<br>**(**Physics of materials for energy and environmental applications**)** | **Technical Session-6**<br>**(**Physics under High Pressure**)** |
| | **Invited talk-7**<br>Amartya Mukhopadhyay,<br>IIT Bombay, Mumbai<br>Layered' transition metal oxides as electrode materials for Na-ion batteries: | **Invited talk-10**<br>Kamil Dziubek, Universität Wien, Austria<br>Pressure-Induced Synthesis Of Heavy Pnictogen Nitrides |
| | **Invited talk**-8<br>Kaustava Bhattacharyya, BARC, Mumbai<br>Heterogeneous Catalysis Perspective towards Energy and Environment: Structural and Mechanistic Understanding. | **Invited talk-11**<br>Rekha Rao, BARC, Mumbai<br>Experimental Observation of Giant Negative Linear Compressibility-A Rare Counter-intuitive Property |
| **12:30-13:00** | **Invited talk-9**<br>Saurabh Lodha, IIT Bombay, Mumbai<br>b-Ga2O3 Devices for High Power Electronics | **Contributory Oral presentations**<br>**a0026, b0019**<br>**(2 nos.)** |
| **13:00-14:00** | **Lunch** | |
| **14:00-15:30** | **Technical Session-7**<br>**(**Soft matter and Bio-physics**)** | **Technical Session-8**<br>**(**Translational research**)** |
| | **Invited talk-12**<br>V.K. Aswal, BARC, Mumbai<br>Structure and Intercations in Reentrant Soft Matter | **Invited talk-15**<br>Harish Barshilia, NAL, Bangalore<br>Ultrathin Multilayered Coatings for Gas Turbine Compressor Blades: Solid Particle Erosion and Corrosion Behaviour at High Temperatures |
| | **Invited talk-13**<br>Prabal Maity, IISc, Bangalore<br>Molecular origin of Branch selectivity in Photosystem II | **Invited talk –16**<br>Sangeeta Kale, DIAT, Pune<br>Engineered tactile sensor arrays for robotic gripper applications |
| | **Invited talk-14**<br>Jitendra Bahadur, BARC, Mumbai<br>Decoding the Nanoscale Middle World "The Heart of Matter and Life": Insights from Synchrotron SAXS | **Invited talk-17**<br>Ravindra Pandey<br>Department of Chemistry, IIT Roorkee<br>From Lipid Membranes to Covalent Organic Frameworks: SFG Insights into Interfacial Organization |
| **15:30 - 16:00** | **Contributory Oral presentations**<br>**h0024, k0050**<br>**(2 nos.)** | **Contributory Oral presentations**<br>**e0025, c0103**<br>**(2 nos.)** |
| **16:00-18:00** | **Tea with Poster Presentation** | |
| | **Poster Presentation: Contributory paper**<br>**(Venue :** ***Gargi Block Foyer*****)** | |
| **19:00-20:00** | **Evening talk –2 (Convocation Hall)**<br>Prof. D. D. Sarma, IISc, Bangalore<br>Phase transitions in VO2 and related compounds: surprises and resolutions | |
| **20:00 onwards** | **Dinner** | |
| **Day 3: Sunday, December 21, 2025** | | |

| | | |
|---|---|---|
| **09:30-11:15** | **Presentations by Young achievers<br>(3 presentations)<br>Venue: (Convocation Hall)** | |
| **11.00-11.30** | **Tea Break** | |
| **11:30-13:00** | **Technical Sessiom-9 (contd.)<br>Presentations by Young achievers<br>(3 presentations)** | |
| **13:00-14:00** | **Lunch Break** | |
| | **APJ-AKB Lecture Hall 1** | **APJ-AKB Lecture Hall 2** |
| **14:00-15:30** | **Technical Session-10**<br>(Physics of Halide Perovskites) | **Technical Session-11**<br>(Emerging magnetic and spintronic material-I) |
| | **Invited talk-18**<br>K. V. Adarsh, IISER, Bhopal<br>Excitonic Correlations and Cooperative Emission in Metal-Halide Perovskites | **Invited talk – 22**<br>S Bedanta, NISER, Bhubaneswar<br>Advancing Organic Spintronics: Interface Engineering and Emerging Effects |
| | **Invited talk-19**<br>Ranjani Viswanatha, JNCASR, Bangalore<br>Spin Physics in Metal Halide Perovskites | **Invited talk – 23**<br>Aftab Alam, IIT Bombay, Mumbai<br>Altermagnetism and its Variants: A New Paradigm in the Field of Magnetism |
| | **Invited talk –20**<br>Manojit Bag, IIT Roorkee<br>Halide Perovskites for Next-Generation Optoelectronics: An Approach Towards Neuromorphic Computing | **Invited talk - 24**<br>Soumya Jyoti Ray, IIT Patna<br>Spin Transport across two-dimensional Spinterfaces |
| **15:30-16:00** | **Invited talk – 21**<br>G D Mukherjee, IISER, Kolkata<br>Is Structural Distortion good for Pb-free Halide Perovskites? | **Contributory Oral presentations<br>j0105, g0018<br>(2 nos.)** |
| **16:00-18:00** | **Tea with Poster Presentation** | |
| | **Poster Presentation: Contributory paper<br>(Venue: APJ – AKB Lecture Hall)** | |
| **19:00-20:00** | **Cultural Function (Convocation Hall)** | |
| **20:00** | **Dinner** | |
| **Day 4: Monday, December 22, 2025** | | |
| **09:30-11:00** | **Technical Session-12<br>Thesis presentation - 3<br>(Venue: Convocation Hall)** | |
| **11:00-11:30** | **Tea Break** | |
| **11:30-13:00** | **Technical Session-12 (contd.)<br>Thesis presentation - 3<br>(Venue: Convocation Hall)** | |
| **13:00-14:00** | **Lunch Break** | |
| **14:00-15:30** | **Technical Session-13**<br>(Physics of Semiconductor Devices)<br>(Venue: APJ AKB Lecture Hall 1) | **Technical Session-14**<br>(Emerging magnetic and spintronic material-II)<br>(Venue: APJ AKB Lecture Hall 2 ) |

| | | |
|---|---|---|
| | **Invited talk-25**<br>Abir De Sarkar, INST, Mohali<br>Insights into Inversion Symmetry Breaking in 2D Materials: Piezoelectricity and Spin-Orbitronics | **Invited talk-28**<br>Subham Majumdar, IACS, Kolkata<br>Spontaneous Anomalous Hall Effect in Some Layered Transition Metal Compounds |
| | **Invited talk-26**<br>Govind Gupta, CSIR-NPL, New Delhi<br>Design and Development of Energy-Efficient Semiconductor Optoelectronic Devices | **Invited talk-29**<br>P D Babu, UGC-DAE-CSR, Mumbai<br>Incommensurate Magnetic Structures and Complex magnetism of Certain Rare Earth Intermetallics |
| | **Invited talk- 27**<br>S Pitale, BARC, Mumbai<br>High Purity Germanium: Key Advances in Single Crystal Growth and Detector Fabrication | **Invited talk-30**<br>A Thamizhavel, TIFR, Mumbai<br>Crystal Electric Field effect in Ce-Based intermetallic compounds |
| **15.30-16.00** | **Contributory Oral presentations**<br>**e0026, d0036**<br>**(2 nos.)** | **Invited talk-31**<br>Surendra Singh, BARC, Mumbai<br>Realization of magnetic helical structure and interface modified exchange interaction in RE-TM multilayers: A polarized neutron reflectivity study |
| **16:00-18:00** | **Tea with Poster Presentation** | |
| | **Poster Presentation contributory paper**<br>**(Venue: APJ AKB Lecture Hall Entrance)** | |
| **19:00-20:00** | **Evening talk –3 (Convocation Hall)**<br>R. Vijayaraghvan, TIFR, Mumbai<br>Observing Quantum Effects In A “Macroscopic” Electrical Circuit: Nobel Prize in Physics 2025 | |
| **20:00 onwards** | **Dinner** | |
| **Day 5: Tuesday, December 23, 2025** | | |
| **09:30-11:15** | **Technical Session-15**<br>**(**Surface and Interface Physics**)** | |
| | **Invited talk – 32**<br>Bivas Saha, JNCASR, Bangalore<br>Metal/Semiconductor Superlattices: Building Matter Layer-by-Layer | |
| | **Invited talk –33**<br>R. B. Tokas, BARC, Mumbai<br>Precision optical multilayer coatings for lasers and photo physical systems: Design and Development | |
| | **Invited talk – 34**<br>Pritam Deb, Tezpur University<br>Out-of-plane heterostructure array as robust electrode for energy storage application | |
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| **13:00-14:00** | **Lunch Break** | |

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# ABSTRACTS

# PLENARY TALKS

**PL-1**

**MAX IV Laboratory – Prospects For Advancing Synchrotron Science Into The 2030s**

Director Olof Karis
*MAX IV Laboratory, Fotongata 2, 224 84 Lund, Sweden*
*olof.karis@maxiv.lu.se*

**Abstract:** MAX IV Laboratory, located in Lund, Sweden, hosts the world's first fourth-generation synchrotron light source — a 3 GeV storage ring based on a pioneering multi-bend achromat (MBA) design. Since its inauguration in 2016, MAX IV has evolved into a highly productive facility, now operating 16 beamlines and serving about 2000 users annually from Sweden, the Nordic region, and beyond.

In this presentation, I will briefly introduce the facility's operational framework, followed by selected examples of recent scientific achievements — including spectroscopy, microscopy, and imaging applications in materials and life sciences.

A key element of MAX IV's long-term strategy is MAX 4U, a planned upgrade of the 3 GeV storage ring that will reduce emittance to below 100 pm·rad through a targeted "surgical" intervention. This will provide enhanced brightness and coherence, particularly relevant for many new application in X-ray science. The upgrade will also enable improved beamline performance and new requirements and opportunities for advanced optics and instrumentation.

**PL-2**

**New scientific opportunities at the European X-ray Free Electron Laser**

Sakura Pascarelli
*Holzkoppel 4, Schenefeld, 22869 Germany*
*sakura.pascarelli@xfel.eu*

**Abstract:** Hard X-ray Free Electron Laser are opening novel avenues in the investigation of fundamental processes in many areas of science, from physics to chemistry, biology and materials science, because they allow investigation of matter at the timescales of electron and nuclear dynamics (down to fs), with chemical selectivity and bulk sensitivity. I will briefly introduce the European XFEL and report on a selection of scientific highlights in different areas of research. Applications address fundamental processes of light-matter interaction, ultra-fast dynamic processes in liquids and solids, investigation of electronic and structural properties and their dynamics in biomolecules, nanostructures, disordered materials and high energy density states of matter.

**PL-3**

**Dirac Fermions in The Presence of Electron Correlation**

Kalobaran Maiti
*Indian Association for the Cultivation of Science, 2A & 2B Raja S. C. Mullick Road, Jadavpur, Kolkata 700032*
*Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai 400005, India*
**Email: kbmaiti@gmail.com*

**Abstract:** Topological insulators are bulk insulators with symmetry protected metallic surface states which exhibit Dirac cone like band dispersions representing particles with no rest mass. The properties of these Dirac fermions in the presence of electron correlation is an interesting emerging area of research as electron-electron Coulomb repulsion usually enhances the effective mass of the particles. So, what happens to the particles with zero rest mass? Rare-earth based systems appear good candidate materials for such study. The first such material, $SmB_6$, identified to be a Kondo insulator, attracted much attention, and found to exhibit exceptional properties [1]. Another Sm-based binary system, SmBi exhibits signature of multiple Dirac cones; gapped and ungapped [2,3]. Employing ultra-high-resolution ARPES, we discover destruction of a surface Fermi surface across the Neel temperature while the behavior of Dirac cones survives across the magnetic transition.

Non-symmorphic systems could be good materials as the Dirac cone at the high symmetry point such as zone boundary becomes robust even in the presence of strong spin-orbit coupling. We find, the Kondo lattice systems, $CeAgSb_2$ and $CeCuSb_2$ exhibit unusual spectral features; the typical Kondo feature is not observed in the electronic structure though the bulk properties show Kondo-type behavior. Instead, we find a new feature in the core level spectra [4,5]. The ARPES data of $CeAgSb_2$ show distinct Dirac cones as well as diamond-shaped nodal lines; the slope of these linear bands is unusually high, larger than that in graphene and maintains its high value in a wide energy range indicating robust high velocity of these relativistic particles [6]. The slope becomes smaller in the vicinity of strongly correlated Ce 4*f* bands forming a kink providing an interesting example of kink due to correlation induced effects.

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[4] Sawani Datta et al. PRB 105, 205128 (2022).
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[6] Sawani Datta et al. Nanoscale 16, 13861 (2024).

**PL-4**

**Magnetic, orbital, ferroelectric, and superconducting orders in $YBa_2Cu_3O_7/Nd_{1-x}(Sr,Ca)_xMnO_3$ multilayers**

Christian Bernhard

*Department of Physics, University of Fribourg, Chemin du Musee 3, CB-1700 Fribourg, Switzerland*

**Email:Christian.bernhard@unifr.ch*

**Abstract:** I will provide an overview of the highlights of our longterm research effort that is aimed at developing a better understanding of the magnetic and electronic properties of multilayers from the high $T_c$ superconductor $YBa_2Cu_3O_7$ (YBCO) and perovskite manganites, like $Nd_{1-x}(Sr,Ca)_xMnO_3$ (NCSMO).

I will start with a brief description of the pulsed laser deposition growth of these multilayers and their structural characterization. Subsequently, I will present the result of a Resonant Inelastic X-ray Spectroscopy (RIXS) study at the Cu_L-edge [1]. In particular, I will focus on the anomalous magnon dispersion of the interfacial $CuO_2$ layer that provides evidence for an altermagnetic order that originates from an orbital and electronic reconstruction that takes place at this interface.

Finally, I will present our recent work on electronic noise rectification that occurs in some of these YBCO/NCSMO multilayers [2]. The underlying ratchet-type electronic potential originates from a competition between different magnetic and electronic order within the NCSMO layers. I will show that the resulting spontaneous voltage (SpV) signals can be rather large (hundreds of millivolt) and readily tuned with a magnetic field. The SpV signal also shows a unique memory functionality that may enable the design of autonomous memory devices that are powered by electronic background noise. I will also comment on the special role played by the thin YBCO layers that cannot fully screen the electric fields which emanate from the NCSMO layers and thus exhibit an activated and non-reciprocal transport behavior. Notably, these YBCO layers become superconducting with a rather high $T_c$ value of about 80K, if a large magnetic field or a high electric current is applied [2].

[1] S. Sarkar *et al.*, PNAS Nexus, Vol. **3**, pgae100 (2024) doi.org/10.1093/pnasnexus/pgae100

[2] M. Soulier *et al.*, Nature Commun., Nat. Commun. **16**, 5900 (2025). https://doi.org/10.1038/s41467-025-61014-7

# EVENING TALKS

**ET-1**

**Research using Indus and possibilities with 4th generation High brightness Synchrotron Radiation source**

Sanjay Kumar Rai

*X-ray Diffraction & Metrology Section, Raja Ramanna Centre for Advanced Technology, Indore*

**Abstract :** Indus 1 and Indus 2 are the only two operating synchrotron radiation sources in India. These sources have been operating in round the clock mode since February 2010 and have been in extensive use by the research community of India. Currently, there are 18 operational beamlines on Indus 2 and 7 on Indus 1 and a few more are are expected to be available for users shortly. The talk will give a flavor of the kind of research being done at Indus-1 and 2. The requirement for a High Brightness Synchrotron Radiation Source (HBSRS) for the Indian scientific community will be explained. How HBSRS will support cutting-edge research in diverse fields like materials science, biology, medicine, and nanotechnology, to foster innovation in indigenous industries. Some details of Indian plan for developing our own HBSRS will be discussed.

**ET-2**

**Phase transitions in $VO_2$ and related compounds: surprises and resolutions**

D. D. Sarma

*Solid State and Structural Chemistry Unit, Indian Institute of Science, Bengaluru 560012, India*

**Email:sarma@iisc.ac.in and sarma.dd@gmail.com*

**Abstract:** Materials in which sudden changes in conductive properties can be induced by external stimuli have attracted attention for decades under the broad heading of metal-insulator transition. An iconic example is vanadium dioxide, $VO_2$. Its metal-insulator transition at $T_c = 340$ K has been rationalized in terms of the accompanying structural transition (rutile-to-monoclinic, R-M1) below which all vanadium atoms pair into dimers, and electronic correlations promote a non-local spin-singlet insulating state. It is also known that the structural aspects and phase transition of pure $VO_2$ can be intriguingly influenced by small (<10%) doping with various elements, such as Al, Cr, and Fe. In addition, $VO_2$ can also exist in many polymorphs besides the most commonly occurring form of R and M1 mentioned above. Together, all these $VO_2$-derived variants encompass a fascinating range of physical phenomena that challenge our understanding of structure-property relationships as well as of metal-insulator transitions. Following an introduction to what we already know, I shall present some of our recent works that underline the surprises of this family of compounds and explain our attempts to understand them.

**ET-3**

**Observing Quantum Effects In A "Macroscopic" Electrical Circuit: Nobel Prize in Physics 2025**

R. Vijayaraghavan

*Tata Institute of Fundamental Research, Dr. Homi Bhabha Road, Colaba, Mumbai 400005*

**Email:r.vijay@tifr.res.in*

**Abstract:** The Nobel Prize in Physics for 2025 has been awarded to John Clarke, Michel Devoret, and John Martinis for conducting a series of experiments that demonstrated quantum tunneling and energy quantization in a "macroscopic" electrical circuit for the first time. In this talk, I will explain the experiments they conducted using a superconducting electrical circuit element called a Josephson junction. I will illustrate how this experiment was a master stroke in both the choice of the system and the clever engineering used to sufficiently isolate it from its environment, enabling the observation of quantum effects. These early experiments set the stage for the development of quantum bits using superconducting circuits, a leading architecture for building practical quantum computers.

# INVITED TALKS

**IT-1**

**Tunable mid-infrared plasmonic metasurfaces**

Ewald Janssens

*Quantum Solid State Physics, Department of Physics and Astronomy, KU Leuven, Belgium*

*e-mail: ewald.janssens@kuleuven.be*

**Abstract:** Metasurfaces are artificial two-dimensional materials with a periodic pattern of subwavelength-scaled structures, the meta-atoms. Metasurfaces can control the properties (amplitude, phase, polarization and momentum) of the light with which they interact. However, most conventional metasurfaces are "passive'', i.e. fixed by the geometric design, and cannot be "actively'' controlled by an external stimulus of thermal, electrical, mechanical, or optical origin. In modern photonics, it is highly desirable to develop real-time actively controllable metasurfaces for advanced applications.

The first part of the talk deals with our recent work on hybrid graphene-metal metasurfaces. Although graphene has exceptional tunable electrical properties, its zero-bandgap nature, low optical absorption (~2.3%), and difficult integration with metallic nanostructures have limited its use in photonic devices. By optimizing the graphene-metal metasurface design and the addition of an alumina barrier layer, we could enhance the real-time plasmonic resonance tuning [1]. Other steps forward were the inclusion of a Fabry-Perot cavity to enhance the light-graphene interaction and the addition of an encapsulating dielectric layer for stable operation in ambient conditions [2]. Bias-controlled reflectance tuning could be further enhanced, reaching modulation depths of 60%, by the reduction of the gaps between neighboring plasmonic antennas. Gaps below 10 nm could be fabricated by combining lift-off, physical vapor deposition, and ion milling techniques [3].

The second part of the talk concentrates on all-optical modulation of plasmonic metasurfaces. The most common method to modulate the optical characteristics of materials is via optical pumping through a semiconductor bandgap, which requires high photon energies. We demonstrated that career multiplication by impact ionization in a silicon substrate following the interaction of the metasurface with sub-bandgap mid infrared radiation strongly modulate the optically transmitted signal on picosecond time scales [4]. These observations are validated through an analytical model and numerical simulations, which clarify the roles of plasmonic field enhancement and impact ionization in shaping carrier dynamics [5]. These findings may trigger applications in low-photon energy ultrafast all-optical modulators.

[1] F. Han, T.L. Pham, X. Zheng, K. Pilarczyk, N.T. Tung, G.A.E. Vandenbosch, J. van de Vondel, N. Verellen, E. Janssens, Advanced Optical Materials 12 (2024) 2303085.

[2] F. Han, K. Pilarczyk, Z. Lin, C. Sun, G.A.E. Vandenbosch, J. Van de Vondel, P. Van Dorpe, X. Zheng, N. Verellen, E. Janssens, Lasers and Photonics Reviews (2025) 2402258.

[3] F. Han, Z. Lin, K. Pilarczyk, H. Tang, G.A.E. Vandenbosch, J. Van de Vondel, X. Zheng, N. Verellen, E. Janssens, Advanced Science e06898 (2025).

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**IT-2**

**Far-Field, Near-Field and Time Resolved Terahertz (THz) Spectroscopy of Materials**

S. S. Prabhu

*Department of Condensed Matter Physics and Material Science, Tata Institute of Fundamental Research, Mumbai 400005, India*

*e-mail: prabhu@tifr.res.in, shriganesh.prabhu@gmail.com*

**Abstract:** Terahertz (THz) spectroscopy offers large opportunities in the ultrafast study of materials of various kinds. There are no cheap and compact high-power sources or sensitive detectors of THz radiation. They are either expensive or difficult to fabricate. Using Laser driven THz sources and detectors, we can build THz time domain spectroscopy (TDS) setup. We have developed several Terahertz (THz) spectroscopic techniques to study different materials from single crystals to metamaterials. We studied THz optical properties of Vanadium doped [100] β-Ga2O3 using THz-TDS.[1] The V-doped β-Ga2O3 crystal shows strong birefringence in the 0.2-2.4 THz range. We measured phase retardation over the whole THz range by developing THz Time-Domain Polarimetry (THz-TDP). It is observed that the V-doped β-Ga2O3 crystal behaves both as a quarter waveplate (QWP) at 0.38, 1.08, 1.71, 2.28 THz, and a half wave-plate (HWP) at 0.74 and 1.94 THz, respectively. [2] We have also studied Metamaterials of different types for various applications. Polarization dependent transmission through an array of subwavelength apertures can have practical applications. Such metasurfaces can be deployed as Intelligent Transmitting Surface (ITS) for 6th Generation (6G) short-range communication. We studied THz transmission through such surfaces. We developed a Near Field Scanning THz Microscope for this purpose. Several interesting Metamaterials were studied using this unique THz Microscope of its kind. Whatever is seen by using Computer simulation, those near field patterns can be observed using this unique microscope.

In topological materials, shielding of bulk and surface states by crystalline symmetries has provided hitherto unknown access to electronic states in condensed matter physics. Interestingly, photo- excited carriers relax on an ultrafast timescale, demonstrating large transient mobility that could be harnessed for the development of ultrafast optoelectronic devices. We systematically characterize the relaxation dynamics of a topologically nontrivial chiral single crystal of PtAl by optical pump probe measurements[3]. Quasiparticles are pumped from the valence band (VB) to the conduction band (CB), leading to a fast non-equilibrium Fermi-Dirac distribution of photo excited carriers. Based on our analysis of experimental data on transient reflectivity and electronic structures, we conclude that the relaxation process involves both acoustic and optical phonons with oscillation frequencies of 0.06 and 2.94 THz, respectively, on the ultrafast timescale before the carriers reach equilibrium through the slow process of quasiparticle recombinations. The second order nonlinear optical response of PtAl has been characterized by second

harmonic generation (SHG). PtAl with a space group of P213 allows only one non-zero susceptibility element i.e. d14, with large value of 468(1) pm/V, which is significantly larger than that observed in standard GaAs(111) and ZnTe(110) crystals. The intensity dependence of the SHG signal in PtAl reveals a non-perturbative origin. Our optical studies of PtAl provide deeper insight into topological states and offer potential applications in ultrafast optoelectronic devices.

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[1] A. Punjal *et al.*, "Terahertz optical properties and birefringence in single crystal vanadium doped (100) β-Ga 2 O 3," *Opt. Mater. Express*, vol. 12, no. 7, p. 2870, Jul. 2022.

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**IT-3**

**A Facility for Studying Condensed Matter Using the Intense MIR Radiation from an FEL**

M. K. Chattopadhyay[1, 2]

*[1]Free Electron Laser Utilization Section, Raja Ramanna Center for Advanced Technology, Indore 452 013, India.*
*[2]Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400 094, India*
*e-mail: maulindu@rrcat.gov.in.*

**Abstract:** After the design, development and successful commissioning of an Infra-red Free Electron Laser (IR-FEL) at RRCAT, a commensurate user facility is being built to facilitate IR-FEL light based experiments. Continuous wavelength tunability of the IR-FEL radiation from 12.5 - 50 $\mu$m has been demonstrated, and more than 10 MW peak out-coupled power and ~30 mW Continuous Wave (CW) average out-coupled power at 21.8 $\mu$m wavelength and 2 Hz macropulse repetition rate (PRR) has been achieved. This translates to a CW average Spectral Brightness ~$2 \times 10^{14}$ photons/s/mm$^2$/mrad$^2$/0.1% BW at the source. In recent experiments, ~14 mW CW average power at a wavelength of 19.12 $\mu$m has been transported up to the experimental stations, which, for 2 Hz PRR, translates to more than 50 $\mu$J energy over the 10 ps width micropulses of the IR-FEL light. The typical spectral width of the IR-FEL radiation measured at the user station is about 1%. The layout of the FEL utilization facility with six user ports has been finalized, and two ports are already in operation where user experiments with the IR-FEL radiation are being performed. Details of the available experimental facilities, plans for the development of more facilities in the near future, and selected experimental results obtained using the IR-FEL light shall be presented.

**IT-4**

**The emerging world of topological semimetals**

Abhirup Roy Karmakar [1] Arghya Taraphder [1] and Gour P Das [2,*]

*[1] Department of Physics, Indian Institute of Technology Kharagpur, W.B.721302, India*
*[2] Research Institute for Sustainable Energy (RISE), TCG Centres for Research and Education in Science and Technology, Sector V, Salt Lake, Kolkata 700091, India.*
**e-mail:gour.das@tcgcrest.org*

**Abstract:** The emergence of topological order in condensed matter physics marks the beginning of a new era in the world of materials. The tone has been set up by some disruptive discoveries, such as Quantum Hall effect, Graphene etc. More recently, topological semimetals have captivated focus due to their intriguing electronic, transport and optical properties as well as application potential in fabricating topological quantum devices. In this talk, I shall first give a brief overview of the Berry curvature induced phenomena in topological semimetals, which came into limelight after the discovery of Graphene. This will be followed by some recent works carried out in our group on two different kinds of magnetic Weyl Semimetals (WSM) viz. (a) anomalous thermal transport in WSM
Co3Sn2S2 [1] and (b) circular photogalvanic effect in WSM CeAlSi [2]

[1] Abhirup Roy Karmakar, S. Nandy, A. Taraphder, G.P. Das *Phys. Rev.* ***B*** **106**, 245133 (2022)

[2] Abhirup Roy Karmakar, A. Taraphder, G.P. Das *Phys. Rev.* ***B*** **111**, 195105 (2025)

**IT-5**

**Boroxol Ring Fraction in $B_2O_3$ Glass**

Debendra Meher, and Nikhil V.S. Avula and Sundaram Balasubramanian*

*Chemistry and Physics of Materials Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur P.O., Bangalore 560064.*
**e-mail:bala@jncasr.ac.in*

**Abstract:** The standard method to model inorganic glasses is to carry out atomistic molecular dynamics (MD) simulations using an empirical force field. While such force fields have evolved much and are mature to describe intermolecular interactions in molecular materials, those for extended networks such as inorganic glasses are not validated to the same degree. The reason is not far to seek. Inorganic systems display greater covalency, changes in oxidation states and coordination than molecular systems -- features which are inherently difficult to capture through force fields. Model-free experimental validation of such simulations too is rather rare for glassy systems. Machine learned potentials (MLP), benchmarked to reproduce quantum density functional theory (DFT) energies and forces are ideally placed to resolve the matter. Herein, MD simulations of $B_2O_3$ glass, using a bespoke MLP are used to address the fraction of boron atoms present in hexagonal boroxol ($B_3O_3$) units. Raman and NMR experiments show this

fraction to be 70%, while empirical MD simulations obtain less than 10%. The current work is able to obtain unprecedented boroxol fractions in the melt-quenched $B_2O_3$ glass, beyond 40%.

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**IT-6**

**Quantum phenomena in planar Josephson junctions**

Narayan Mohanta
*Department of Physics, Indian Institute of Technology Roorkee, Roorkee 247667, India.*
*e-mail: narayan.mohanta@ph.iitr.ac.in*

**Abstract:** Planar Josephson junctions are heterostructures, made of semiconductor/superconductor multi-layers, which provide a platform for electrons to move in a two-dimensional plane. In this talk, I'll discuss various quantum phenomena that these platforms can exhibit, such as a robust Josephson effect, topological superconductivity and superconducting diode effect. Emergent topologically-protected quasi-particles, such as Majorana bound states, can be realized in a topological superconducting phase and these states can be used to build topological qubits which are building blocks of fault-tolerant quantum computation. I'll also discuss about superconducting diode effect which can be realized without any external magnetic field in these platforms. Our theoretical results are expected to stimulate and guide experimental studies to explore various quantum phenomena and to realize next-generation devices for technological applications.

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**IT-7**

**'Layered' transition metal oxides as electrode materials for Na-ion batteries: Composition - Structure - Environmental stability - Electrochemical behaviour/performance**

Amartya Mukhopadhyay
*Advanced Batteries and Ceramics Laboratory, Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Mumbai, India*
*e-mail: amartya_mukhopadhyay@iitb.ac.in*

**Abstract:** 'Layered' transition metal (TM) oxides are a fascinating class of materials, whose properties can be suitably tuned in a variety of ways; such as, by selecting TM-ions/dopants having preferred electronic configurations, engineering the crystallographic site occupancy by dopants, controlling/modifying the degree of covalence of TM-O bonds, modifying lattice spacing(s), tuning phase assemblage etc. Such modifications done from the fundamental perspectives influence the performances of TM-oxides for a variety of applications, including their widespread usage as cathode-active materials in alkali metal-ion batteries. In the context of the Na-ion battery system, O3-type 'layered' Na-TM-oxides are promising as cathode-active materials due to their inherently high initial Na-content (as compared to the P2 counterparts); but suffer from instabilities caused due to multiple phase transformations during Na-removal/insertion and sensitivity to air/moisture. Against this backdrop, by tuning the overall covalency of the cation-oxygen bonds in the TM-layer (which, in turn, influences the Na-O bond) and also with the help of a dopant having d0 electronic configuration (viz., no OSPE), we have been able to tune the composition and structural features to suppress the phase transitions upon Na-removal/insertion and improve the air/water-stability in significant terms; so much so that long-term cyclic stability has been achieved with health/environment-friendly 'aqueous processed' electrodes (sans, usage of toxic/expensive chemicals like NMP and PVDF) [J. Mater. Chem. A 8 (2020) 18064, Adv. Energy Mater. 13[19] (2023) 2204407, J. Mater. Chem. A 13 (2025) 5807]. The changes in structural features, which have led to such outstanding water-stability, include differential contraction/dilation of the Na-'inter-slab'/TM-'slab' spacing and partial occupancy of the dopant at tetrahedral sites of the structure. The former aspect has also been invoked to enhance the Na-transport kinetics and, hence, the rate-capability of the, otherwise, inherently sluggish O3-structured cathode material [ChemComm 59 (2023) 4332]. Furthermore, in the context of the more 'rate-

capable' P2-structured 'layered' Na-TM-oxide cathode materials, but which lack in terms of a lower starting Na-content (typically, ~0.67 Na-ions p.f.u.), a universal strategy towards designing and developing high Na-containing P2-structured 'layered' Na-transition metal oxides has been evolved. This is based on raising the average 'charge:size' ratio of the cation-combination in the TM-layer and concomitant TM-O bond covalency, resulting in lower effective negative charge on O-ions; and, in turn, rendering the prismatic coordination of O-ions around Na-ions more favourable even at higher Na-content. Accordingly, by careful selection of the combination of non-TM-/TM-ions in the TM-layer, a high Na-containing (viz., ~0.84 p.f.u.) P2-type Na-TM-oxide has been developed, which, as a cathode material for Na-ion batteries, exhibits a high reversible sodiation capacity of ~151 mAh/g (@ C/5; within 2-4 V vs. Na/Na+), exceptional cyclic stability pertaining to ~98% capacity retention after 500 galvanostatic cycles @ 2.5C and also stability upon exposure to air/water [Chem. Mater. 34 (2022) 10470]. Activation of anionic redox raises the capacity to close to ~193 mAh/g (i.e., within 2-4.5 V vs. Na/Na+), while still maintaining good stability compared to other state-of-the-art O-redox based cathodes.

**IT-8**

**Heterogeneous Catalysis Perspective towards Energy and Environment: Structural and Mechanistic Understanding.**

K. Bhattacharyya
*Chemistry Division, Bhabha Atomic Research Centre, Mumbai*
*e-mail: kaustava@barc.gov.in*

**Abstract:** The structure-sensitive catalytic properties of small-sized particles are relevant for both metal and non-metal catalyst surfaces. Change in the electron density as a function of particle size causes a disparity in chemical properties, results in different binding modes of the adsorbate molecules than that which is observed in corresponding bulk materials. Different structural parameters like oxidation state, particle size, band gap etc. play different and significant roles to alter the photocatalytic activity of the catalyst. Equivalently different surface intermediates are being produced depending on alteration of the surface, source of irradiation and reaction conditions leading to modification in the efficiency and the final product of the photocatalyst. Change in the electron density as a function of particle size causes a disparity in chemical properties, results in different binding modes of the adsorbate molecules than that which is observed in corresponding bulk materials. Different structural parameters like oxidation state, particle size, band gap etc. play different and significant roles to alter the photocatalytic activity of the catalyst.

Equivalently different surface intermediates are being produced depending on alteration of the surface, source of irradiation and reaction conditions leading to modification in the efficiency and the final product of the photocatalyst. The feasibility of the detection of the surface intermediates by spectroscopic tools allows for delineation of reaction route followed during the photo-catalytic processes. The mechanistic understanding for the surface intermediates produced and the related structural attributes leads to better understanding of the catalyst and the catalytic process and in its own turn subjects to evolve a catalyst with better properties and efficiency for the designated reactions.

Some typical results for CO2 reduction (for Renewable Energy) under ambient conditions and in the absence of hydrogen will be discussed in details along with their structure activity correlation. Also degradation of certain VOC and dyes (Environmental Sector) will be understood under the light of both thermal and photocatalytic degradation using suitable catalysts. The role of the different intermediates affecting the reaction mechanism will also be understood as correlated to structure and shape of catalysts.

**IT-9**

**β-Ga2O3 Devices for High Power Electronics**

Saurabh Lodha
*Department of Electrical Engineering, IIT Bombay, Powai, Mumbai, India, 400076*
*e-mail: slodha@ee.iitb.ac.in*

**Abstract:** In recent years, β-Ga2O3 has emerged as a promising semiconductor for high power electronics due to its large and direct bandgap of 4.8 eV that enables a large critical electrical field strength of 8 MV/cm.

This talk will present some of our recent work on β-Ga2O3 gate stacks, Schottky diodes and MOSFETs. Specifically, results for an Al2O3/SiO2 bilayer dielectric gate stack with a low Dit interface [1] and an Al2O3/AlN/SiO2 stack demonstrating tunable, positive flatband voltage through charge trapping in the AlN layer for enhancement mode operation [2] will be discussed. Further, Schottky diode data showing the benefits of improved surface passivation of β-Ga2O3 using a sequence of Ar/O2 plasma and an HF clean [3], an interfacial ultra-thin AlOx layer [4] and with high-k dielectrics such as BZN [5] leading to increased VBR reaching nearly 600 V on 2e16 cm-3 doped epi-layer substrates, will be presented. Finally, we will share the first report of monolithic bi-directional lateral MOSFETs on β-Ga2O3 [6].

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**IT-10**

**Pressure-Induced Synthesis Of Heavy Pnictogen Nitrides**

Kamil Filip Dziubek[1,*], Matteo Ceppatelli[2], Manuel Serrano-Ruiz[2], Marta Morana[3], Demetrio Scelta[2], Roberto Bini[4], Maurizio Peruzzini[2]

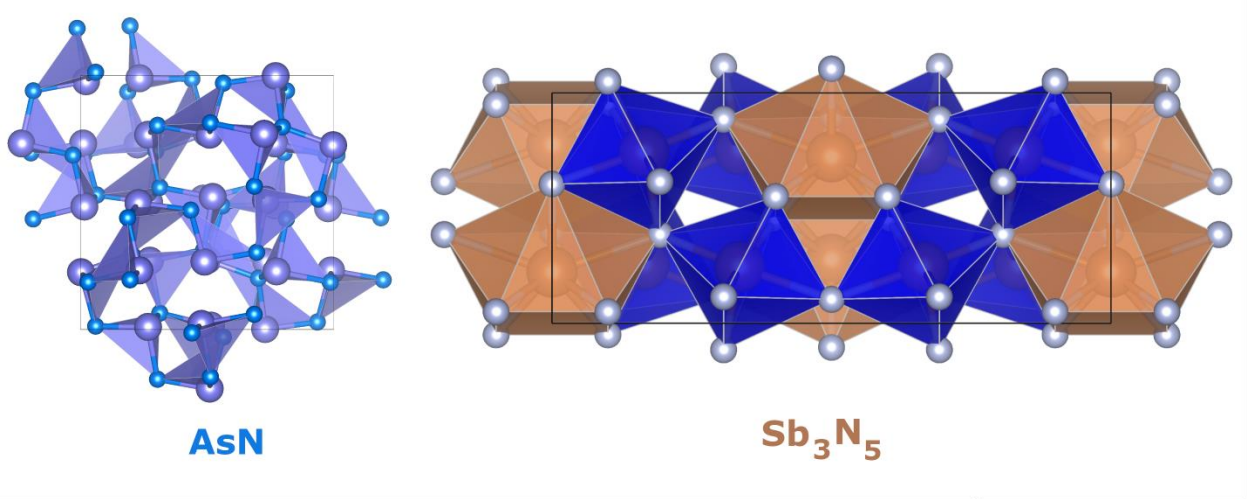
[1]Institut für Mineralogie und Kristallographie, Universität Wien, 1090 Wien, Austria; [2]Institute of Chemistry of OrganoMetallic Compounds, National Research Council of Italy, 50019 Sesto Fiorentino (FI), Italy; [3]Dipartimento di Scienze della Terra, Università degli Studi di Firenze, 50121 Firenze, Italy; [4]Dipartimento di Chimica "Ugo Schiff", Università degli Studi di Firenze, 50019 Sesto Fiorentino (FI), Italy

**e-mail:kamil.dziubek@univie.ac.at*

**Abstract:** Nitrides are binary inorganic compounds known for their diverse mechanical, electronic, and energetic properties, which make them useful in a wide range of applications. Many nitrides are recognized for their exceptional hardness, high melting points and thermal stability. Moreover, they can display valuable electronic and optical properties. However, the synthesis of nitrides can be challenging, which poses a significant limitation to their widespread use.

New nitrides of group 15 elements (pnictogens) have been synthesized under high-pressure high-temperature conditions. Until recently, only two crystalline phases of $P_3N_5$ were discovered, and no crystalline nitrides of arsenic, antimony, or bismuth had been known. Laser heated diamond anvil cells (LH-DACs) allow access to a wide range of high pressure and high temperature thermodynamic conditions, facilitating direct synthesis of binary compounds from the elements. Recently this method led to the synthesis of AsN, $Sb_3N_5$, and BiN, as well as new phases of $P_3N_5$ and $PN_2$.

These results highlight the effectiveness of LH-DACs in facilitating direct chemical reactions between nitrogen and heavier pnictogens, which marks a significant breakthrough in the synthesis of crystalline pnictogen nitrides. The discovery of new phases such as AsN, $Sb_3N_5$, and BiN represents a fundamental advancement in our understanding of group 15 chemistry, providing the evidence that pnictogens heavier than phosphorus can form compounds with nitrogen. This finding opens the door to exploring a new class of advanced materials, which have important implications for fundamental inorganic chemistry and potential technological applications.




**IT-11**

**Experimental Observation of Giant Negative Linear Compressibility-A Rare Counter-intuitive Property**

Rekha Rao[1,2]

*[1]Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India.*

*[2] Homi Bhabha National Institute, Mumbai 400094, India.*

*e-mail: rekhar@barc.gov.in*

**Abstract:** Most materials contract in all crystal directions under hydrostatic compression showing positive linear compressibility. However, in rare cases, some materials expand along one or more crystal directions, demonstrating negative linear compressibility (NLC) or negative area compressibility [1-5]. Most of the materials that display NLC either have very weak NLC or have a very narrow pressure range of structural stability [2-4]. However, we have discovered giant NLC in orthorhombic CuCN over an unusually large pressure range, an extremely rare occurrence. Our experimental studies confirmed this remarkable giant NLC and identified the phonon vibrations responsible for NLC. In this talk, I will present a limited review of experimentally discovered NLC materials, mechanisms proposed; our experimental observation [1] of NLC in CuCN and its mechanism.

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**IT-12**

**Structure and Intercations in Reentrant Soft Matter**

V.K. Aswal
*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400 085, India*
*e-mail: vkaswal@barc.gov.in*

**Abstract:** Reentrant soft matter describes systems where a change in an external parameter (e.g. temperature, concentration, or ionic strength) causes a phase transition, followed by a return to the initial phase [1]. This reentrant behavior is driven by the interplay of different interactions, often including attractive and repulsive forces between particles, as well as interactions with the surrounding medium. Understanding these interactions is crucial for controlling the structure and properties of these materials [2]. The charged colloids represent a model system, where well-established colloidal theories such as Debye-Hückel (DH) theory and/or DLVO theory can be implemented to predict the phase behavior. Recently, reentrant phase transitions in a wide range of colloids (e.g. inorganic and organic nanoparticles, polymers, and biomolecules) have been observed, which are not consistent with these theories. We have looked into the colloid-polymer/multivalent-ions systems, demonstrating such a phase transition in terms of interparticle interactions using small-angle neutron scattering and other supporting techniques [3-11]. It has been shown how the tuning of interparticle interactions from repulsive to attractive and back to repulsive using external parameters leads to reentrant phase behavior. The properties of the reentrant phase are found to be unusually quite different from those of the original phase. For example, reentrant-charged colloids show unprecedented stability against the conventional salt effect and the heat-induced protein denaturation in the reentrant phase may be completely suppressed.

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**IT-13**

**Molecular origin of Branch selectivity in Photosystem II**

Prabal K Maiti
*Center for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore 560012, India*
*e-mail: maiti@iisc.ac.in*

**Abstract:** Photosynthesis, the fundamental process sustaining life on Earth, depends on the Photosystem II (PSII) reaction center's ability to initiate the charge transport process. Using multi-scale simulation methodologies, we have investigated this charge transport process with a focus on the dissimilarity between the two branches of the PSII reaction center, D1 and D2. Utilizing Marcus theory, we have calculated the reorganization energies and activation barriers for all the key steps involved in the charge transport process. Our analysis reveals that while both D1 and D2 branches exhibit similarities in the initial stages, the rate-determining step in the D2 branch has a significantly higher activation barrier (0.2 eV) than D1 branch (0.1 eV), suggesting a much less favorable energetic landscape. Further, the calculation of current-voltage (I-V) characteristics confirms the higher resistance in the D2 branch compared to the D1 branch, emphasizing its non-conductive nature.

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**IT-14**

**Decoding the Nanoscale Middle World "The Heart of Matter and Life": Insights from Synchrotron SAXS**

Jitendra Bahadur[1,2]
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai, 400085, India*

[2]*Homi Bhabha National Institute, Mumbai, 400094, Mumbai, India*
**e-mail: jbahadur@barc.gov.in*
**Abstract:** Understanding how matter organizes between molecular and mesoscopic length scales remains a central challenge across condensed matter and soft-matter physics. This intermediate "middle world" is where collective interactions, emergent order, and hierarchical structuring first appear which governs mechanical, optical, and transport properties in both advanced materials and biological systems. Synchrotron-based Small-Angle X-ray Scattering (SAXS) offers a uniquely powerful window into this regime, enabling in situ, in operando, and time-resolved characterization at nanometer length scale in wide range of research areas including soft-matter assemblies, biomolecular complexes, hybrid nanostructures, and functional materials. The talk will highlight the key features and capabilities of the SAXS beamline at Indus-2 synchrotron. It will be shown how the synchrotron SAXS allows us to unravel self-assembly pathways in multi-component colloids with a particular emphasis on the formation mechanisms of hierarchically structured colloidal assemblies directed by cooperative interactions resulting in cluster formation, coacervation, and mesoscale ordering. Self-assembly is a fundamental bottom-up route to constructing complex, hierarchical soft-matter structures, where subtle colloidal interactions dictate the emergent morphology of the resulting superstructures. In multi-component colloidal systems, intrinsic heterogeneity and interactions spanning multiple length scales generate rich physical behavior, dynamic self-organization, and pronounced sensitivity to small external stimuli driven by a delicate balance of enthalpic and entropic forces. Controlling the assembly of colloids into organized structures through electrostatic complexation with oppositely charged polyelectrolytes results in interesting phase diagrams and their tunable interactions and response to external stimuli enable controlled self-assembly into complex structures. Ultimately, these insights reveal why the nanoscale "middle world" is not merely a structural bridge, but the origin of emergent physical properties central to materials science, soft matter, biophysics, and condensed matter research.
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**IT-15**

**Ultrathin Multilayered Coatings for Gas Turbine Compressor Blades: Solid Particle Erosion and Corrosion Behaviour at High Temperatures**

Harish C. Barshilia* and Venkataramana Bonu
*Surface Engineering Division, CSIR-National Aerospace Laboratories, Bangalore - 560 017*
**e-mail: harish.nal@csir.res.in*
**Abstract:** When an aircraft operates in deserts, dusty environments, or marine regions, solid particles and sea salt accelerate towards the gas turbine compressor and cause severe damage to compressor blades (typically made of Ti6Al4V alloy) [1-3]. Several investigations led to the conclusion that the physical vapour deposition (PVD) based surface protective coatings are holistic solution to the problem [1-3]. Accordingly, solid particle erosion (SPE) and corrosion-resistant nanolayered TiCr/TiCrN multilayer coating (~9 μm thick) was developed on Ti6Al4V using a semi-industrial magnetron sputtering system. The TiCr/TiCrN coating contains three stacks of TiCr/TiCrN bi-layers (bi-layer thickness ~7.3 nm) separated by two energy-absorbing TiCr layers. The average SPE resistance of the coating is 93 times higher than bare Ti6Al4V at 30 m/s and 300 °C (ASTM-G76-18) [4]. The coating also showed excellent erosion resistance from room temperature up to 500 °C. In terms of corrosion resistance, the coated Ti6Al4V exhibited ~two orders of magnitude better corrosion protection than bare Ti6Al4V in 3.5 wt.% NaCl solution and successfully passed ASTM-B117 salt spray tests [4]. The high density of interfaces with varying elastic modulus and grain orientations in the coating helped in blocking corrosive media and erosion crack penetration. The other important high-cycle fatigue tests were also conducted and found that a 30% drop in endurance limit of Ti6Al4V after the coating [5], which is a usual trend after deposition of a hard coating; a similar 30% drop in the endurance limit of Ti6Al4V was reported by NASA after deposition of erosion resistant coating [6]. After 9 minutes of erosion pre-damage, bare Ti6Al4V lost ~28% of fatigue life, whereas coated Ti6Al4V lost only ~7% [5]. Thus, despite an initial endurance penalty, the coating significantly mitigates SPE-induced fatigue degradation. The TiCr/TiCrN coating was also deposited on a compressor impeller made of Al-7075 and successfully tested in a small gas turbine engine (NJ5-PT04) while passing alumina erodent feed of ~55–60 g/min at ~100,000 rpm. The thrust, mass flow, and RPM reduced significantly for the uncoated impeller due to severe erosion of the leading edges. In contrast, the coated impeller maintained stable thrust, mass flow, and RPM, and exhibited no significant erosion damage during the test. Overall, the TiCr/TiCrN nano-multilayer coating offers

strong erosion resistance, excellent corrosion protection, and significantly suppresses SPE-induced fatigue deterioration, demonstrating its suitability for compressor blade applications.

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**IT-16**

**Engineered tactile sensor arrays for robotic gripper applications**


Sangeeta N. Kale[1,*], Akshara R.[1], M Ghaisas[1], Revathi S.[1], K. Akella[2], J. Pednekar[2], S.E. Talole[2]

[1]*Department of Applied Physics Defence Institute of Advanced Technology, Pune, INDIA*

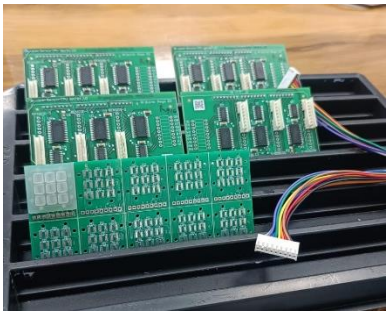
[2]*Research and Development Establishment Engineers (RDEE – DRDO), Pune, INDIA*

**e-mail:sangeetakale2004@gmail.com*



**Abstract:** Environmentally-unsafe locations require robotic intervention for surveillance and rescue operations. These include locations which are deployed with chemical and biological weapons, gas chambers, areas with landslides or earthquake or even fire sites. Such robotic or autonomous systems require multiple sensors; of which the tactile sensors are most crucial. While numerous studies focus on sensors for low and moderate pressure ranges, there is an increasing demand for devices capable of operating in a wide pressure range without compromising sensitivity, linearity, or durability. Most importantly, these sensors must be compatible with standard mass production procedures, moving beyond solely laboratory-based fabrication. To address this challenge, we must develop well-engineered sensor arrays which could be installed on the robotic gripping fingers. These should be able to identify the objects (without vision) and lift/move the object without crushing / breaking / slipping.

Through this presentation, various polymer composite systems will be discussed on which our group has extensively worked to develop a complete sensor-array system used for robotic 3-finger gripper applications in defence. Materials such as TPU (Tetra Poly urethane) and PDMS (polydimethylsiloxane) are used as the basic matrix in which additives such as f-MWCNTs (functionalized multi-walled carbon nanotubes) are added to get the desired piezo-resistive performance. The range of pressure-handling capacity of these sensors is carefully controlled using two parameters; namely the sensor porosity and the percentage of the additive fillers. Considering the percolation-threshold, the filler concentration was varied between 4 – 7% to cover and pressure handling capacity from as low as 0.1 N to about 30 N. 4 mm3 sensor units were fabricated and packaged in a 3 x 3 matrix array format. Such 3 arrays were installed on 3 fingers of a robotic gripper. Grasping of the object and "slip-detection with re-grasping" was realized using appropriate hardware-software interface and python programming. The engineering aspects, performance details (sensitivities, accuracy, repeatability and recovery) will be discussed in detail. A tactile sensing system, ready to be deployed, will be elaborated.

**IT-17**

**From Lipid Membranes to Covalent Organic Frameworks: SFG Insights into Interfacial Organization**


Ravindra Pandey

Department of Chemistry, *Indian Institute of Technology Roorkee, Roorkee 247667, India.*

*e-mail: rpandey@cy.iitr.ac.in*



**Abstract.** Vibrational sum-frequency generation (SFG) spectroscopy, an interface-specific probe of molecular organization and hydrogen-bonding, reveals striking parallels in interfacial dynamics across biomembranes and covalent organic framework (COF) synthesis. In the first part of my talk, I will discuss human serum albumin (HSA) interactions with phospholipid monolayers (dDPPC and dDPPG) at the air–water interface. At pH 3.5, HSA deeply penetrates liquid-expanded (LE) membranes via electrostatic and hydrophobic forces, markedly increasing lipid chain order. Penetration is strongly suppressed in tightly packed liquid-condensed (LC) phases and in zwitterionic dDPPC, demonstrating that proteins dynamically modulate membrane fluidity and ordering, with implications for cellular signaling and lipid-based biomaterials. In the next part, in situ SFG monitored light-

driven synthesis of 2D COF thin films at the same air–water interface. Real-time spectra show that photoactivated imine condensation induces pronounced ordering and strengthened hydrogen bonding of interfacial water as crystalline domains emerge, whereas non-photoactivated reactions produce amorphous films with disordered water structure. Supported by MALDI and MD simulations, interfacial water thus serves as a sensitive probe of crystallinity during COF growth.
These combined studies highlight SFG's unique ability to connect protein-driven membrane restructuring and water-templated framework crystallization, unifying molecular-level understanding of biological and materials interfaces.
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**IT-18**
**Excitonic Correlations and Cooperative Emission in Metal-Halide Perovskites**
K. V. Adarsh
*Department of Physics, Indian Institute of Science Education and Research, Bhopal 462066, India*
*e-mail:adrash@iiserb.ac.in*
**Abstract:** Metal-halide perovskites (MHPs) have emerged as an exceptional class of quantum materials that bridge the domains of semiconductor physics and molecular dynamics. Their remarkable electronic and optical tunability arises from a delicate interplay between charge, spin, and lattice degrees of freedom. In this talk, I will discuss how this interplay governs excitonic (bound electron-hole) phenomena in MHPs from tightly bound excitons and exciton–polaron coupling to the formation of correlated many-body states such as exciton condensation and superfluorescence. Recent ultrafast spectroscopic studies reveal that dynamic lattice fluctuations and strong electron–phonon coupling stabilize coherent excitonic populations even at room temperature, enabling collective light–matter phases previously restricted to cryogenic regimes. I will also highlight how structural attributes such as facet engineering, dimensional confinement, and compositional tuning allow the emergence of cooperative emission and amplified spontaneous emission with ultralow thresholds. Finally, I will outline the outstanding challenges and opportunities of these materials for coherent quantum light sources, electrically driven superfluorescent lasing, and room-temperature quantum photonic technologies.

**IT-19**
**Spin Physics in Metal Halide Perovskites**
Ranjani Viswanatha
*Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore, India, 560064*
*e-mail:rv@jncasr.ac.in*
**Abstract:** Over the last decade, metal halide perovskites have emerged as excellent materials for various energy applications owing to their superb properties such as long carrier diffusion length, strong spin orbit coupling and large absorption coefficient. While they have been extensively studied by several optical techniques, little is known about their spin electronic structure despite being probable candidates for spintronics applications. Spin physics provides high precision tools for addressing the electronic states in the vicinity of the band gap. In this talk, I plan to discuss their spin electronic structure using magnetic circular dichroism and density functional theory. Observation of Rashba splitting in multi-layer $Cs_2PbI_2Cl_2$ 2D Ruddlesden-Popper Phase (RPP) perovskite nanocrystals (NCs) induced by chemical strain will be discussed. Magnetic circular dichroism (MCD) measurements reveal significant Zeeman splitting, indicating strong spin-orbit coupling. CD, PL, XRD and Raman data along with density functional theory (DFT) are used to study the origin of this splitting. Investigation of the influence of chemical strain on asymmetry-induced phenomena, such as the Rashba effect in $Cs_2PbI_2Cl_2$ NCs, highlight their potential as promising platform for advanced technologies.

**IT-20**
**Halide Perovskites for Next-Generation Optoelectronics: An Approach Towards Neuromorphic Computing**
Tanuj Kumar, Mohit Kumar, Ramesh Kumar and Monojit Bag*
*Department of Physics, Indian Institute of Technology Roorkee, Roorkee 247667, India.*
**e-mail:monojit.bag@ph.iitr.ac.in*
**Abstract:** Hybrid halide perovskites have been the materials of this decade due to their exceptional optoelectronic semiconducting properties. These materials are widely used in solar photovoltaics, light-emitting diodes, lasers, sensors and detectors, as well as energy storage applications. Very recently, they have also been used in other electronic devices such as field-effect and electrochemical transistors. However, electrolyte-gated FETs are sparse due to the instability of halide perovskites in commonly used electrolytes. Here, we demonstrate a methodology to enhance the stability of halide perovskites in a three-terminal electrochemical field-effect transistor geometry. An ion-selective membrane has been introduced between a quasi-solid-state gel electrolyte and the active perovskite layer to prevent direct contact with the solvent. The drain current can be modulated by modulating both the gate voltage and photo-illumination. We have fabricated mixed-input switchable universal logic gates by

selectively tuning the channel conductivity. This is one of its first kinds where the logic operation has been demonstrated for electronic and optical inputs simultaneously. Therefore, these devices can be the next generation of neuromorphic computing.

**IT-21**

**Is Structural Distortion good for Pb-free Halide Perovskites?**

Goutam Dev Mukherjee
*Department of Physical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur – 741246.*
*e-mail:goutamdev@iiserkol.ac.in*

**Abstract:** In recent times the exploration of energy-harvesting materials for photovoltaic and optoelectronic applications has inspired intense research interest in the scientific community. In this search, halide-Perovskites have shown excellent photovoltaic properties. In this talk I shall take examples of a few lead-free model halide Perovskites and double Perovskites and show that structural distortions enhance the photoluminescence (PL) in these systems. The structural distortions are induced in the samples by using high pressure techniques and then studied the materials using various experimental tools, such as, x-ray diffraction, Raman spectroscopy, Photoluminescence measurements and absorption spectroscopy.

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Ref. 2: Structural transition and emission enhancement in vacancy-ordered halide double perovskite Cs2TeCl6 under pressure, Suvashree Mukherjee et. al., Appl. Phys. Lett. **126**, 141901 (2025).
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**IT-22**

**Advancing Organic Spintronics: Interface Engineering and Emerging Effects**

Subhankar Bedanta
*Laboratory for Nanomagnetism and Magnetic Materials (LNMM), School of Physical Sciences, National Institute of Science Education and Research (NISER), An OCC of Homi Bhabha National Institute (HBNI), Jatni 752050, Odisha, India*
*e-mail: sbedanta@niser.ac.in*

**Abstract:** Interface induced phenomenon in ferromagnetic/organic semiconductor is an emerging topic towards organic spintronics [1,2]. Buckminsterfullerene ($C_{60}$) is a potential candidate for organic spintronics due to many desirable properties viz. low spin orbit coupling, large spin diffusion length at room temperature etc. It has been observed that $C_{60}$ exhibits ferromagnetism at the interface of FM/$C_{60}$ [3-5]. We have prepared single layers of Fe, Co and CoFeB, and compared the magnetic properties to the bilayers of Fe/$C_{60}$, Co/$C_{60}$ and CoFeB/$C_{60}$. The films were prepared on both MgO (001) and Si (100) substrates. Finite magnetic moment was obtained in the $C_{60}$ layer at the interface between the Fe/$C_{60}$ and Co/$C_{60}$ layers by polarized neutron reflectivity measurements [3-5]. Magneto optic Kerr effect (MOKE) based microscopy was performed to observe the effect of the magnetic $C_{60}$ layer on the hysteresis loop shape and the domain images of the FM (Fe, Co, CoFeB, NiFe) layers [3-7]. We also study the change in magnetic anisotropy due to the presence of spinterface in these bilayer systems [4-7]. It has been found that anisotropy increases with $C_{60}$ thickness. We have also studied the FM/OSC having perpendicular magnetic anisotropy (PMA). In this context we have taken Pt/Co/$C_{60}$ as a model system. It has been observed that introducing a $C_{60}$ layer increases the anisotropy and decreases the domain size of the system [8]. Further we also show that ferromagnetism can be observed at the interface between Cu/$C_{60}$ interface. In this case due to the charge transfer from Cu to $C_{60}$, density of states of Cu gets modified which leads to ferromagnetism in Cu [9]. We will also discuss how DMI can emerge at the spinterface between Co/$C_{60}$ interface [10]. At the end I will discuss the role of interface in enhancing the spin pumping in a CFB/β-W/$C_{60}$ and CFB/$Alq_3$ systems [11-14].

**Acknowledgement:** I sincerely express my thanks to my collaborators for their active participation and various funding agencies for the generous financial support.

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**IT-23**

**Altermagnetism and its Variants: A New Paradigm in the Field of Magnetism**

Bishal Das,[1] Jadupati Nag,[1,2] Chanchal K Barman,[3] Sayantika Bhowal,[1] Akio Kimura,[4] K. G. Suresh[1], **Aftab Alam**,*[1]
[1]*Department of Physics, IIT Bombay Powai, Mumbai – 400076, Maharashtra India*
[2]*Department of Materials Science and Engineering, & Materials Research Institute Pennsylvania State University, Pennsylvania 16802, USA*
[3]Dipartimento di Fisica, Universit`a di Cagliari, Cittadella Universitaria, Monserrato (CA) 09042, Italy
[4]*Research Institute for Semiconductor Engineering (RISE), Hiroshima University, 1-4-2 Kagamiyama, Higashi-Hiroshima 739-8527, Japan*
**e-mail:aftab@phy.iitb.ac.in*

Spintronics has emerged as a promising alternative to conventional electronics, driven by the discovery of topological phases with protected spin-polarized states and by new magnetic materials exhibiting unconventional spin-splitting phenomena. Among these, *altermagnetism*—a recently recognized phase of collinear antiferromagnets—has attracted considerable attention for its unique momentum-dependent spin polarization arising from non-relativistic origins.

Traditionally, altermagnets are classified via spin group formalism based on opposite-spin sublattice transformations involving rotations or reflections, but excluding inversion or translation. While this framework merges ferrimagnets with ferromagnets, we also propose yet another distinct subclass of ferrimagnets—termed *Alter-Ferrimagnets*—which exhibit alternating momentum-dependent spin-polarized bands within the Brillouin zone, even in the presence of multiple magnetic species. In this talk, I will discuss the microscopic origin of these unconventional magnetic phenomena and present candidate materials that realize both altermagnetism and alter-ferrimagnetism. Combined theoretical and ARPES studies reveal the coexistence of altermagnetism with topological features, offering new insights into the interplay between magnetism and topology.

**IT-24**

**Spin Transport across two-dimensional Spinterfaces**

Soumya Jyoti Ray
*Department of Physics, IIT Patna, Bihta 801103*
*e-mail:ray@iitp.ac.in (Email of corresponding author)*

**Abstract:** Two-dimensional (2D) materials have brought fresh prospects for spintronics, as evidenced by the rapid scientific progress made in this frontier over the past decade. In particular, for charge perpendicular to plane vertical magnetic tunnel junctions, the 2D crystals present exclusive features such as atomic-level thickness control, near-perfect crystallography without dangling bonds, and novel electronic structure-guided interfaces with tunable hybridization and proximity effects, which lead to an entirely new group of spinterfaces. Such crystals also present new ways of integration of atomically thin barriers in magnetic tunnel junctions and an unprecedented means for developing composite barriers with atomic precision. All these new aspects have sparked interest for theoretical and experimental efforts, revealing intriguing spin-dependent transport and spin inversion effects. Here, we discuss some of the distinctive effects observed in ferromagnetic junctions with prominent 2D crystals such as graphene, hexagonal boron nitride, and transition metal dichalcogenides and how spinterface phenomena at such junctions affect the observed magnetoresistance in devices. Finally, we discuss how the recently emerged 2D ferromagnets bring upon an entirely novel category of van der Waals interfaces for efficient spin transmission and dynamic control through exotic heterostructures.

**IT-25**

**Insights into Inversion Symmetry Breaking in 2D Materials: Piezoelectricity and Spin-Orbitronics**

Abir De Sarkar[a,b]
[a]*Institute of Nano Science and Technology (INST), Knowledge City, Sector 81, Manauli, Mohali, Punjab – 140306, India*
[b]*Department of Physics, Indian Institute of Technology (IIT), Ropar, Punjab-140001, India*
*e-mail:*

**Abstract:** Breaking of inversion symmetry leads to the emergence of several important properties in 2D materials, such as piezoelectricity, valleytronics and spintronics. For instance, HfN2 monolayers [1] exhibit valleytronic properties complementary to those in single-layer MoS2, while the conflux of valley Hall effect, Rashba effect and piezoelectricity is observed in Janus MXSiN2 (M=Cr, Mo, W; X=S, Se, Te) [2], h-NbN and h-TaN monolayers [3]. Out-of-plane piezoelectricity is induced at the interfaces of 2D semiconducting planar monolayers, which show in-plane piezoelectricity individually and zero out-of-plane polarization/piezoelectricity, such as GaN and boron monophosphide (BP) monolayers [4]. The understanding reached in GaN/BP van der Waals heterobilayers (vdWHs) has been reinforced on MoS2/BP [5] and MoSSe/BP vdWHs [6]. Experimental verification of these theoretical predictions is encouraging. The origin of negative piezoelectricity at the interfaces of 2D dialkali oxide and chalcogenide monolayers has been elucidated [7] together with strain tunability in ultrahigh shear piezoelectricity in superflexible non–van der Waals graphitic ScX monolayers (X = P, As, Sb) [8]. Ferroelectricity in AlXY (X=S, Se; Y=Cl, Br, I) monolayers [9] will be presented along with sliding ferroelectricity in ZrX2 (X = Cl, Br, I) bilayers [10].

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**IT-26**

**Design and Development of Energy-Efficient Semiconductor Optoelectronic Devices**

Prof. Govind Gupta[1,2]
[1]*Sensor Devices & Metrology Group, CSIR - National Physical Laboratory (CSIR-NPL), Dr K. S. Krishnan Road, New Delhi 110012, India*
[2]*Academy of Scientific & Innovative Research (AcSIR), CSIR-HRDC Campus, Ghaziabad, Uttar Pradesh 201002, India*
*e-mail: govindnpl@gmail.com, govind@nplindia.res.in*

**Abstract:** Atomically thin materials exhibit unique intrinsic properties that can be modified in various ways. We synthesize a range of atomically thin metal oxides, mono- and dichalcogenides, and nitride materials using solid and vapor phase techniques tailored for specific applications. We have successfully developed neuromorphic sensors through defect engineering and explored using hybrid materials to enhance electronic and optical performance. Additionally, we have created ultra-thin layers that function as self-powered photodetectors, capable of sensing a full spectrum of light from deep ultraviolet to mid-infrared. Recent efforts have focused on understanding the effects of defects and strategies for passivation in monolayer transition metal dichalcogenides, especially regarding their applications in optoelectronics and chemical sensors. By adopting a cross-disciplinary approach, we leverage the multifunctionality of these innovative material systems to address technological challenges faced by industry partners across various sectors, facilitating the integration of advanced materials and functionalities into their products.

**IT-27**

**High Purity Germanium: Key Advances in Single Crystal Growth and Detector Fabrication**

Shreyas Pitale
*Crystal Technology Section, Technical Physics Division, Bhabha Atomic Research Center, Mumbai, India 400 085*
*e-mail: spitale@barc.gov.in*

**Abstract:** High-Purity Germanium (HPGe) is one of the most advanced semiconductor material used for precision radiation detection, providing unmatched energy resolution in gamma-ray spectroscopy. Due to its excellent carrier mobility, high atomic number, and superior energy resolution compared to other semiconductor materials, HPGe is the material of choice for gamma radiation detectors for a wide range of applications, especially in environmental monitoring, nuclear waste management, and radiation safety at the Department of Atomic Energy (DAE). Therefore, our ongoing development of these detectors is essential to meet the growing demands of DAE's research programs.

This talk will provide a comprehensive overview of the current work in the Technical Physics Division (TPD), BARC, focusing on both the crystal growth and detector fabrication aspects of HPGe technology. The first part of the talk will cover the challenges and innovations in germanium crystal growth, primarily using the Czochralski technique to meet the demands of controlled dislocation densities, uniform structural quality and impurity levels. To put it into perspective, achieving the level of purity required for these crystals means reducing impurity concentrations to the parts-per-billion (ppb) range, with net electrically active impurity levels as low as $10^{9}$–$10^{10}$ $cm^{-3}$. This is a level of purity that is rarely achieved in any material, making HPGe crystals among the most pure and sought-after materials for radiation detection applications.

The second part will highlight efforts in fabricating high-performance HPGe detectors. This includes the fabrication processes for cutting, shaping, polishing, and contact formation (using lithium diffusion and boron ion implantation), as well as surface passivation demonstrating the potential of our in-house processes for producing operational detectors adhering to the strict material contamination control. The fabrication chain and its influence on operational parameters will be discussed, along with typical results achieved and lessons learned in process reproducibility. The talk will provide an end-to-end perspective on HPGe detector development, elucidating the synergies between materials science, semiconductor fabrication and radiation detection physics. Attendees will gain insight into the key challenges (impurity control, defect reduction, contact design, and quality assurance) and the strategies we have developed to address them, ultimately contributing to the development of HPGe detectors for future high-precision scientific experiments.

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**IT-28**

**Spontaneous Anomalous Hall Effect in Some Layered Transition Metal Compounds**

Tamali Roy, Mohamad Numan and Subham Majumdar*

*School of Physical Sciences, Indian Association for the Cultivation of Science, 2A and B Raja S. C. Mullick Road, Jadavpur, Kolkata 700 032*

**e-mail: sspsm2@iacs.res.in*

**Abstract:** Quasi two-dimensional layered magnetic materials, in presence of strong spin-orbit coupling, and electron-electron correlation, serves as a platform of studying intriguing electronic and magnetic phenomena. Here we report a rarely observed incident of spontaneous anomalous Hall effect in such two layered compounds, $TbMn_6Sn_6$ and $Fe_{0.27}TaS_2$ in absence of any applied magnetic field.

$TbMn_6Sn_6$ is a layered Kagome magnet with a relatively high ferromagnetic Curie temperature of 423 K. Upon cooling under a moderate magnetic field, the sample attains a magnetization value nearly equal to the saturation magnetization. When subsequently heated in a very small magnetic field, or even under zero field, the sample retains this large magnetization indicating the presence of thermo-remanent magnetization (TRM). This TRM eventually drops sharply around 200 K, exhibiting an ultrasharp transition. A similar behavior is observed in the Hall resistivity, which maintains its saturation value upon heating in zero field after field cooling. The ultrasharp jump in magnetization is clearly mirrored in the Hall data. The observed thermo-remanent behavior in both magnetization and Hall resistivity within the arrested state can be attributed to strong uniaxial anisotropy and the possible presence of a cluster-glass-like phase. The spins ultimately become de-arrested near 200 K through a sharp transition, driven by the weakening of magnetic anisotropy and enhanced thermal fluctuations.

$Fe_{0.27}TaS_2$, on the other hand, is a van der Waals material, where Fe has been intercalated between the van der Waals gap of two $TaS_2$ layers. This composition, like $TbMn_6Sn_6$, also shows TRM upon cooling under a moderate magnetic field of 500 Oe or higher. Remarkably, the thermoremanence persists in zero magnetic field up to temperatures as high as 160 K, well above the ferromagnetic Curie temperature ($T_C$ = 90 K) of the sample. The origin of the TRM in this compound can be attributed to the strong Ising-like spin character and the quasi-two-dimensional nature of the system. Magnetization analysis reveals the presence of short-range magnetic correlations, manifested as a Griffiths singularity extending up to approximately $2T_C$. The TRM is further reflected in a pronounced anomalous Hall effect (AHE) observed even in zero magnetic field. In contrast to the TRM, which persists well above $T_C$, the thermoremanent Hall effect disappears immediately upon heating above $T_C$, suggesting that the emergence of the AHE requires the presence of long-range magnetic order.

The observed thermoremanence in $TbMn_6Sn_6$ and $Fe_{0.27}TaS_2$ can be attributed to the magnetocrystalline anisotropy present in the sample, which itself arises from the Ising character of the spins. Both the compounds show strong uniaxial magnetic anisotropy with the crystallographic *c* axis being the easy axis. On cooling in a positive magnetic field applied along the *c* axis, the spins will get oriented along the *c* direction of easy axis. On removal of the magnetic field, the sample does not get demagnetized immediately because of the presence of free-energy barrier between up and down spins, and the sample retains its magnetization even when temperature is increased. This thermoremanence is responsible for the observed AHE in absence of externally applied magnetic field in $TbMn_6Sn_6$ and $Fe_{0.27}TaS_2$.

**IT-29**

**Incommensurate Magnetic Structures and Complex magnetism of Certain Rare Earth Intermetallics**

P. D. Babu

*UGC-DAE Consortium for Scientific Research, Mumbai Centre, 246-C, CFB, BARC Campus, Trombay, Mumbai - 400085*

*e-mail: pdbabu@csr.res.in*

**Abstract:** Rare-earth (R) and transition metallic (T) compounds have been extensively studied and some of them, especially the reare-earth rich side are known to exhibit highly complex magnetism. Of these the rare-rich compounds of $R_3T$ type exhibit very rich magnetic phenomena, multiple magnetic transitions with temperature, field induced magnetic transitions, etc. The magnetization in many of these systems does not saturate even in magnetic fields up to 150 T. Additionally, some of these compounds having Tb, Ho, Dy, etc., as R atoms have huge magnetic moments of 10 $\mu_B$/atom or above, are thought to be promising magnetocaloric materials as well. Further, there is a large inter-atomic distance between T atoms of the order of ~4˚A or so in these systems, which allows one to explore effect of high pressures on their magnetism as high pressure can significantly alter $f - d$ hybridization between R and T atoms. This presentation will discuss the experimental results on the magnetism of some of the rare-rich compounds and determination of incommensurate magnetic structures that these compounds display. Experimental results of ac & dc magnetization, heat capacity and temperature and field dependent neutron diffraction will be presented. Some results of high-pressure magnetic studies and magnetocaloric effect at ambient and under high pressure conditions will also be discussed.

**IT-30**

**Crystal Electric Field effect in Ce-Based intermetallic compounds**

A. Thamizhavel
*Department of Condensed Matter Physics and Materials Science*
*Tata Institute of Fundamental Research, Mumbai-400 005*
*e-mail: thamizh@tifr.res.in*

**Abstract:** The unique magnetic and electronic behaviors of f-electron systems, particularly those containing lanthanide and actinide ions, have long fascinated condensed matter physicists due to their rich interplay of localized and itinerant electronic states. Among the most critical phenomena governing these systems are the crystal electric field (CEF) effects, which arise from the electrostatic potential created by the surrounding lattice environment acting on the localized f-electron orbitals. These interactions lift the degeneracy of the Hund's rule ground-state multiplets, resulting in a series of well-defined energy levels that crucially determine the macroscopic physical properties of the material. The resulting CEF level scheme dictates the occupation of f-electron states at different temperatures, influencing the system's thermodynamic, magnetic, and spectroscopic responses. In the case of rare-earth intermetallic compounds, the 4f electrons are typically well localized, leading to pronounced CEF-induced anisotropies in their magnetic and electronic behavior. The CEF effects often compete or cooperate with other fundamental interactions such as the Kondo effect and Ruderman–Kittel–Kasuya–Yosida (RKKY) exchange, giving rise to complex ground states including heavy fermion behavior, quantum criticality, and unconventional magnetism. This presentation will focus on the influence of crystal electric field interactions in Ce-based intermetallic compounds, specifically $CeMg_3$, $CeAg_2Ge_2$, and $CeRh_6Ge_4$. These systems provide an excellent platform for investigating the intricate balance between localized 4f moments and their hybridization with conduction electrons. In $CeMg_3$, the cubic environment leads to a well-defined CEF splitting that governs its low-temperature magnetic anisotropy and magnetization behavior. $CeAg_2Ge_2$, with its tetragonal crystal symmetry, exhibits a quasi-quartet ground state which is unusual. Meanwhile, $CeRh_6Ge_4$ presents a more complex scenario, where CEF effects interplay with strong electronic correlations, leading to unconventional magnetic properties.

**IT-31**

**Realization of magnetic helical structure and interface modified exchange interaction in RE-TM multilayers: A polarized neutron reflectivity study**

Surendra Singh
*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai, 400094*
*e-mail:surendra@barc.gov.in*

**Abstract:** The magnetic interaction at interfaces between different ferromagnetic materials can be modified by exploiting interface morphology, which subsequently can be utilised to engineer materials with magnetic properties that are significantly different from the bulk. The rare-earth/transition-metal (RE/TM) ferromagnetic (FM) multilayers are a classic example, where a strong antiferromagnetic (AFM) exchange coupling at interfaces can lead to novel magnetic states and phase transitions between them. The compensated RE-TM heterostructures and alloy films are intensively investigated because of their possible promising applications in the field of all-optical switching, and magnetic storage devices with high speed and density [1]. Recently the realization of a twisted helical magnetic structure with planar 2π DWs and highly correlated magnetic domains in Gd/Co multilayers [2-4] were reported. We found exchange bias in this system below a compensation temperature (Tcomp). We also observed antisymmetric magnetoresistance (MR) at Tcomp, which is in contrast to earlier findings of similar effects in magnetic heterostructures with perpendicular magnetic anisotropy. Using spin dependent specular and off-specular polarized neutron reflectivity (PNR), we observed a twisted helical magnetic structure with planar 2π domain wall (DW) and highly correlated magnetic domains in a Gd/Co multilayer. Here, we discuss the influence of interface morphology on the interfacial exchange interaction and thus on macroscopic magnetization properties of Gd/Co and Gd/Ni multilayer [2-7]. Specular XRR and PNR were used to characterize the depth dependent structure and magnetic properties of the multilayer, which suggested formation of thin alloy layer at interfaces on annealing the multilayer at 573 K. PNR results suggested that the alloy layer is ferromagnetic at room temperature.

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**IT-32**

**Metal/Semiconductor Superlattices: Building Matter Layer-by-Layer**

Bivas Saha

*International Centre for Materials Science & Chemistry and Physics of Materials Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore, 560064, India.*
*e-mail: bsaha@jncasr.ac.in*
**Abstract:** Since the 1960s, the quest to engineer artificially structured materials has driven efforts to combine metals and semiconductors at the nanoscale to unlock novel quantum functionalities. Early metal/dielectric multilayers revealed intriguing tunnelling and optical properties but lacked atomic-scale interface control. To overcome this, we developed the first epitaxial, single-crystalline metal/semiconductor superlattices based on rocksalt nitrides, featuring atomically sharp, defect-free interfaces that exhibit hyperbolic optical behaviour and unusual thermal transport phenomena.
Building on this foundation, we have now demonstrated a new class of epitaxial lattice-matched metal/semiconductor superlattices that transcend conventional structural constraints by integrating refractory hexagonal transition metals with wide-bandgap III-nitride semiconductors. Exemplified by Hf/AlN superlattices, these systems achieve coherent atomic-layer epitaxy and, for the first time, exhibit cross-plane thermionic emission alongside enhanced Seebeck coefficients from carrier energy filtering. These advances establish metal/semiconductor superlattices as a versatile platform for exploring interface-driven quantum phenomena and developing next-generation metamaterials and energy-conversion technologies.
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**IT-33**
**Precision optical multilayer coatings for lasers and photo physical systems: Design and Development**
R. B. Tokas
*Atomic and Molecular Physics Division, Bhabha Atomic Research Centre-400085, Mumbai*
*e-mail: rbtokas@barc.gov.in*
**Abstract:** Optical multilayer coatings are fundamental to the performance of modern laser systems and photo physical experiments. These coatings, composed of alternating dielectric layers, enable precise control of reflection, transmission, and absorption across a broad spectral range. This talk will provide an overview of the principles behind designing and developing multilayer coatings, including quarter-wave and non-quarter-wave stacks, as well as graded-index layers. Special attention will be given to the tailoring of optical and morphological properties of various dielectric materials to meet the specific requirements of different laser wavelengths and experimental conditions. Key challenges in the design of multilayer coatings will be discussed, including laser-induced damage thresholds, stress management, and environmental stability, with a focus on low-scatter devices for high-power laser applications. Material selection, deposition techniques, and in-situ monitoring will be highlighted as essential factors in the development process. The talk will also cover some of the developed precision-customized multilayer devices, such as polarization-dependent grazing incidence broadband anti-reflection coatings, broadband high-reflective mirrors, large-area silica-protected metallic mirrors, laser output couplers, etc. These case studies will demonstrate how tailored coatings are realised in real world, high-performance laser applications.

**IT-34**
**Out-of-plane heterostructure array as robust electrode for energy storage application**
P. Deb
*Advanced Functional Materials Laboratory, Tezpur University (Central University), Tezpur 784028, India.*
*e-mail: pdeb@tezu.ernet.in*
**Abstract:** The development of advanced electrode material functioning efficiently in energy storage technology offers a promising route for next-generation energy storage systems. However, conventional in-plane structures often face challenges including short-circuiting and limited accessibility of electroactive sites during charge–discharge processes. Contrarily, out-of-plane heterostructure array provides rapid charge transport across vertically arranged nanoflakes, and forms less heat pockets due to less contact area between vertically arranged ensembles. Importantly, such structures are not only providing improved heat dissipation efficiency, but also reducing the degradation of electrode material during the prolonged charging/discharging process, signifying the out of-plane structures ideal for harsh environment. In addition, application of magnetic fields holds great potential for future energy storage technologies by enabling more efficient ion transport and interfacial charge control, ultimately leading to enhanced performance and energy efficiency with minimal additional power input.

# CONTRIBUTORY PAPERS

# a) Phase transitions and dynamics

**a0001**

**Gamma Irradiation and Thermal Cycling Effects on Transformation Behavior of Heat-Treated NiTi Shape Memory Alloys**

Murari M S[1*], Rahina M K[2], Swaroop K[3], Gururmurthy S C[4], Yashodhara I[5]

[1]*NITTE (Deemed to be University), Nanoscience Research Laboratory, Department of Physics, NMAM Institute of Technology, Nitte, Karkala 574110, Karnataka, India*

[2]*Dept. Of Materials Science Mangalore University Mangalagangotri, Mangalore 574199, India*

[3]*Department of Physics, School of Mathematical and Physical Sciences, GM University, Davanagere 06, Karnataka, India*

[4]*Department of Physics, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka 576104, India*

[5]*Department of Physics, Ramaiah Institute of Technology, Bengaluru-54, Karnataka, India*

**Email:murarims.pape@nitte.edu.in*

NiTi-based shape memory alloys (SMAs) are extensively used in aerospace, biomedical, and nuclear applications due to their distinctive phase transformation behaviour, including the shape memory effect and superelasticity. However, their functional stability under gamma irradiation and thermal fatigue remains a key concern for deployment in extreme environments. This study investigates the influence of gamma irradiation (0, 20,40,60 and 80 kGy) and thermal cycling on the transformation behaviour of NiTi SMAs heat-treated at 660 °C. Samples were subjected to gamma irradiation and repeated thermal cycling, and their transformation temperatures—martensite start ($M_s$), martensite finish ($M_f$), austenite start ($A_s$), and austenite finish ($A_f$) were measured using Differential Scanning Calorimetry (DSC). Results indicate minimal change in transformation temperatures across irradiation doses, with only a slight variation in $A_s$ and $A_f$. This suggests that the 660 °C heat treatment effectively stabilizes the microstructure against radiation-induced defects. Thermal cycling revealed a gradual decrease in transformation temperatures during the initial cycles, attributed to dislocation accumulation and internal stresses. After approximately N=7 cycles, transformation temperatures stabilized, and the appearance of the R-phase was observed in all irradiated samples. These findings confirm that NiTi SMAs, when properly heat-treated, maintain phase transformation characteristics even after moderate gamma exposure and repeated thermal cycling. This highlights their potential for reliable performance in applications requiring structural adaptability and radiation tolerance, such as actuators in nuclear facilities, aerospace components, and implantable medical devices.

**a0002**

**Impact of $BiFeO_3$-Induced Structural Disorder on Phase Transitions in $KNbO_3$: A Neutron Diffraction Study**

Debaprasad Nayak[1],S. K. Mishra[1,2,*], and P. S. R. Krishna[1]

[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India.*

[2]*Homi Bhabha National Institute, Anushaktinagar Mumbai 400094, India.*

**Email:debaprasad@barc.gov.in*

This study investigates the structural phase transitions in the $0.9KNbO_3$–$0.1BiFeO_3$ (KB10) solid solution using detailed Rietveld refinement of temperature-dependent neutron diffraction data. The strongest changes in the diffraction patterns occur around ~ 62° at provides evidence for structural phase transitions at these temperatures. The analysis reveals that KB10 undergoes a sequence of phase transitions distinct from those observed in undoped $KNbO_3$. Specifically, the material exhibits a transition from a ferroelectric orthorhombic phase (Amm2) to a ferroelectric tetragonal phase (P4mm) near 450 K, followed by a transformation to a paraelectric cubic phase (Pm-3m) around 675 K. These transition temperatures are notably lower than those of pure $KNbO_3$, which transitions from orthorhombic to tetragonal at 498 K and from tetragonal to cubic at 708 K. The observed shifts in phase stability underscore the significant influence of $BiFeO_3$ doping on the structural and ferroelectric behavior of $KNbO_3$, offering insights into the design of tunable lead-free ferroelectric materials and opens exciting possibilities for developing novel energy storage devices.

**a0003**

**Signature of Magnetic Excitations in Quasi-One-Dimensional Spin Chain Orthovanadate $BaCu_2(VO_4)_2$**

Swayam Kesari[1,*], Rekha Rao[1,#] and S. N. Achary[2]

[1]*Solid State Physics Division,* [2]*Chemistry Division, Bhabha Atomic Research Centre, Mumbai 400085, India.*

[*] *Email: swayam@barc.gov.in(Email of corresponding author)*

[#] *Email: rekhar@barc.gov.in(Email of corresponding author)*

Signature of magnetic excitations in a Quasi-One-Dimensional Spin Chain compound $BaCu_2(VO_4)_2$ has been investigated by using Raman spectroscopy down to 4.8K. The Raman spectra of $BaCu_2(VO_4)_2$ previously unreported, is reported by us at ambient and at several low temperatures. The changes observed in the line shape of the Raman bands and behaviour of the background profile in the Raman spectra below 60K indicates signature of magnetic excitations.

**a0004**

**Ga Doping Induced Tailoring of Electrical Properties in $Ge_2Sb_2Te_5$ Thin Films**

Neeru Bala[1] and Anup Thakur[2,*]

[1]*Department of Applied Sciences, Chitkara University Institute of Engineering and Technology, Chitkara University, Jhansla, Rajpura, Patiala, Punjab 140401, India*

[2]*Advanced Materials Research lab, Department of Physics, Punjabi University, Patiala-147002, Punjab, India*

**Email: dranupthakur@gmail.com(Email of corresponding author)*

The study investigates the current voltage (I-V) characteristics of as-deposited and annealed (160 ℃ and 260 ℃) Ga-doped $Ge_2Sb_2Te_5$ thin films, with a thickness of 200 nm. In comparison to the undoped GST thin film, Ga doping concentrations up to 10 % increased the current by two orders of magnitude. The current in the as-deposited and annealed (160 ℃ and 260 ℃) Ga-GST thin film ranged from μA to mA, verifying the phase transition from amorphous to crystalline. For 10 % Ga-doped GST thin films, a reduction in electrical resistance by an order of tens was observed, thereby facilitating lower programming current requirements for memory applications. With annealing treatment Ga-doped GST thin films allow controlled tuning of charge transport, leading to reduced power consumption and improved suitability of doped composition for energy-efficient phase-change memories.

**a0005**

**Structural Evolution of Wolframites under Compression**

Siddhi Garg[1,*], K. K. Pandey[1,2], Ashok K. Verma[1,2], Daniel Errandonea[3], H. K. Poswal[1,2], Nandini Garg[1,2]
*[1]High-Pressure and Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400085, India*
*[2]Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*
*[3]Departamento de FísicaAplicada-ICMUV-MALTA Consolider Team, Universidad de Valencia, C/Dr. Moliner 50, 46100 Burjassot, Valencia, Spain*
** Email: siddhi@barc.gov.in*

The high-pressure behaviour of a molybdate (β-$ZnMoO_4$) and a tungstate ($NiWO_4$) was investigated using powder x-ray diffraction and Raman spectroscopy up to ~45GPa. Both of these compounds crystallize with the monoclinic wolframite structure (P2/c) at ambient conditions. However, their structural behaviour under high pressure is quite different. $ZnMoO_4$ undergoes a first order reversible structural phase transition near 40 GPa to a monoclinic Cm phase, accompanied by an increase in Mo coordination. Whereas, $NiWO_4$ retains both its symmetry and coordination even after the phase transition above ~ 27 GPa in which a tripling of its unit cell was observed. Raman spectroscopy corroborates these transitions, showing abrupt intensity changes and new modes in β-$ZnMoO_4$ around 39 GPa, and peak broadening in $NiWO_4$ beyond 27GPa.The comparison of their structural behaviour allows us to understand the influence of transition metal cations and polyhedral compressibilities in determining phase stability and transition pathways in wolframite-type tungstates and molybdates under compression.

**a0006**

**Effect of High-Pressure Plastic Deformation on Ge**

Vaishnavi Sharma[1], K. K. Pandey[1,2,*], Rahul Kaiwart[1,2], H. K. poswal[1,2]
*[1]High Pressure and Synchrotron Radiation Physics Division,*
*Bhabha Atomic Research Centre, Mumbai 400085, India*
*[2]Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*
**Email:kkpandey@barc.gov.in*

We explored the effect of high-pressure severe plastic deformation on germanium using rotational diamond anvil cell and synchrotron based in situ scanning micro-XRD measurements. We observed nearly threefold reduction in the cubic diamond to β-tin phase transition (PT) initiation pressure, from ~ 10.4 GPa under quasi-hydrostatic conditions to ~ 3.1 GPa under severe plastic deformation at high pressures. The PT initiation pressure is found to be independent of pressure-shear pathways. The phase fraction of β-tin phase increases with further plastic deformation at same load conditions, suggesting primary role of the accumulated plastic strain for this PT. The PT completion pressure however increases slightly from ~12.7 GPa to ~13.6 GPa under plastic deformation. These findings provide the first in situ evidence of plastic strain–driven phase transformation in germanium and emphasize the critical role of deviatoric stresses in shaping phase behavior in covalently bonded materials.

**a0007**

**Prediction and Studies of New High Pressure Phase in $Th_4H_{15}$**

Saiyad M. A. S[1, 2] and Ashok. K. Verma[1, 2]
*[1]Bhabha Atomic Research Center High Pressure & Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India. [2]Homi Bhabha National Institute, Mumbai 400085, India*
*Email:saiyadmas@barc.gov.in*

In this work, we predict and characterize a pressure-induced first-order phase transition of $Th_4H_{15}$ from ambient cubic to a tetragonal structure at 24 GPa and 0 K, using ab initio simulations with GGA functionals. By evaluating the relative changes in enthalpy between the two structures, we identify a sharp enthalpy crossover accompanied by a discontinuous volume change, indicating a first-order phase transition. The equilibrium lattice constants, bulk moduli, band structure, density of states and partial density of states are calculated. While both the structure retain their metallic character, significant changes are observed in density of states and band structure which may affect conductivity and the superconducting behaviour. Our calculated lattice constant and bulk modulus for BCC structure are consistent with previous theoretical and experimental studies. We also calculated critical temperature of BCC structure which is in good agreement with the experimental data.

**a0008**

**Theoretical Insights Into Phase Behavior Of Surfactant-DNA Complexes Based On Lattice Electrostatics**

Amit Kumar Majhi[1,*]

[1]Gour Mohan Sachin andal Mahavidyalaya, Bireshwarpur, South 24 Parganas, West Bengal, 743336, India
*Email: kumaramitmajhi@gmail.com
We present a theoretical model to analyze phase stability in DNA-surfactant complexes via electrostatic energy calculations. By evaluating micelle-DNA and micelle-micelle interactions within square, hexagonal, and super-hexagonal lattices using linearized Poisson-Boltzmann theory, we predict stable structures under varying micelle sizes and ionic strengths. Our results explain experimental phase transitions observed in DTAB and MTAB systems, establishing a framework for rational design of polyelectrolyte-surfactant assemblies.

**a0010**

**Hund's Coupling Induced Metal-Insulator Transition in the Spin-1/2 Falicov-Kimball Model on A Triangular Lattice**

Swati Pandey*, Umesh K. Yadav and Pradip K. Priya
*Department of Physics, Ewing Christian College, Prayagraj - 211002*
**Email: pandey14swati@gmail.com*
Role of Hund's coupling on the spin-1/2 Falicov-Kimball Model on a triangular lattice is explored, employing the numerical calculation and classical Monte-Carlo simulation technique. In the ground state, configurations from regular Neel ordered antiferromagnetic pattern to ferromagnetic or mixed phases of both are observed and exhibit a metal to insulator transition with variation of Hund's coupling at different onsite Coulomb correlation strength. It is noted that d-electrons density varies significantly with Hund's coupling and plays vital role in the phase transition in the system. These results are applicable to systems like $GdI_2$, $NaTiO_2$ and $NaVO_2$ etc. and useful to develop sensors and high energy storage devices.

**a0011**

**High-Pressure High-Temperature Structural Investigation on $Gd_2Zr_2O_7$:Sm**

Rahul Kaiwart[1, 2, *], M. Modak[1], A. Dwivedi[1], Santosh K. Gupta[3], K. K. Pandey[1, 2], and H. K. Poswal[1, 2]
*[1]High Pressure & Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India.*
*[2]Homi Bhabha National Institute, BARC Training School Complex, Anushaktinagar, Mumbai 400094, India.*
*[3]Radiochemistry Division, Bhabha Atomic Research Centre, Mumbai 400085, India.*
**Email:rkaiwart@barc.gov.in*
$Gd_2Zr_2O_7$ with 0.5% Sm doping crystallizes in defect fluorite structure (space group: Fm-3m) at ambient conditions. Synchrotron based high pressure x-ray diffraction experiments at room temperature were conducted upto ~48 GPa. The compound undergoes structural transformation at ~21 GPa. The high pressure phase can be described as orthorhombic type structure (space group: Pnma). However, when the compound, compressed at ~21 GPa was simultaneously subjected to laser heating at 1500ºC, it undergoes structural transformation to the monoclinic structure. Therefore, we propose that orthorhombic is rather a meta-stable phase. We have also performed photoluminescence (PL) measurements on $Sm^{3+}$ under compression at room temperature and immediately after the laser heating. PL measurements on heated sample reveal more Stark components of $^4G_{5/2} \rightarrow {}^6H_{7/2}$ transition, indicating a lower symmetry of the high-pressure phase than the orthorhombic structure. The transformation is irreversible upon release of pressure.

**a0012**

**Finite-temperature STLS Study of Dynamical Dielectric Response of Warm-dense Electron Gas**

Priya Arora[1] and R. K. Moudgil[1,*]
*[1]Department of Physics, Kurukshetra University, Kurukshetra – 136 119, Haryana (India)*
**Email:rkmoudgil@kuk.ac.in*
We present a theoretical study of the dynamical dielectric response and plasmonic excitations in the warm-dense three-dimensional homogeneous electron gas (3DHEG) at the Fermi temperature, employing the finite-temperature extension of the Singwi-Tosi-Land-Sjölander (STLS) approach. Specifically, we compute the frequency and wavenumber dependent dielectric function $\varepsilon(q,\omega)$ and the imaginary part of inverse dielectric function $\mathrm{Im}[\varepsilon^{-1}(q,\omega)]$, quantities directly relevant to X-ray Thomson scattering experiments. Particular emphasis is placed on analyzing the zeros of $\mathrm{Re}[\varepsilon(q,\omega)]$, which determine the plasmon dispersion and damping characteristics. By benchmarking against the recent path-integral Monte Carlo (PIMC) simulations due to Dornheim*et al*., we demonstrate that in the weak coupling regime, the STLS quantitatively captures essential correlation-driven effects such as the position and broadening of the plasmon peak, which are otherwise significantly misrepresented by the (lower-order) Random Phase Approximation (RPA). As the coupling strength increases, the STLS continues to follow the plasmon flattening and enhanced damping, although its quantitative accuracy gradually diminishes. These findings establish the STLS approach as a reliable theoretical framework for modeling dynamical screening and collective excitations in warm-dense matter, providing notable improvements over conventional mean-field theories.

**a0013**

**Investigating the structural phase transition of α(2H)$In_2Se_3$**

Saswata Talukdar, Suvodeep Paul, Devesh Negi, Suraj Saini, Shalini Badola, and Surajit Saha[a)]
*Indian Institute of Science Education and Research Bhopal,462066, India*
*[a)]Corresponding author: surajit@iiserb.ac.in*

In recent years, the complex characteristics and polymorphic nature of indium selenide ($In_2Se_3$) distinguish it as a prominent candidate among 2D semiconductors for memory and nano-electronic applications. Despite comprehensive research on its thermal, electrical, and optical properties, the structural dynamics, especially the phase transitions generated by temperature, remain enigmatic. Temperature-dependent Raman spectroscopy of bulk α(2H) $In_2Se_3$ reveals clear signatures associated with the structural transition from the α to β-phase. In comparison, Raman measurements on exfoliated flakes highlight a pronounced thickness-dependent modulation of the transition behavior, underscoring the critical role of dimensionality in governing phase stability and evolution. On the other hand, low-temperature photoluminescence experiments indicate significant alterations in optical emission, providing insights into carrier dynamics and defect-level recombination. This work elucidates the phase behaviour and optoelectronic characteristics of $In_2Se_3$, which is crucial for its incorporation into forthcoming nanoscale electronics.

**a0014**

**Thermochromic Characterization of Hydrothermally Synthesized $VO_2$ Films for Smart Radiative Devices**

Aniruddha Mondal[1, *], Arka Dey[1] and Iman Biswas[1]
[1]*Department of Physics, National Institute of Technology Durgapur, Durgapur 713209, India*
**Email:aniruddhamo@gmail.com*

Vanadium dioxide ($VO_2$) exhibits a semiconductor-to-metal transition (SMT) near room temperature, making it a promising material for thermochromic applications. In this work, $VO_2$ films were fabricated via hydrothermal synthesis, spin coating, and annealing. Structural and morphological studies confirmed the formation of crystalline monoclinic $VO_2$ (B) with uniform grain distribution. A custom-designed chamber enabled in situ transmittance measurements, revealing a clear thermochromic response with a reduced phase transition temperature ($T_{SMT}$) of 53.8 °C. Electrical measurements showed nearly two orders magnitude of resistance change, with $T_{SMT}$ at 66.05 °C. The strong optical and electrical switching behavior confirms the suitability of the films for smart radiative coatings.

**a0015**

**Strength Properties of Tungsten Carbide (WC) under Dynamic Loading**

D. Mukherjee[1]*, S. Gandhi[1], A. S. Rav[1] and K. D. Joshi[1,2]
[1]*Applied Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, India*
[2]*Homi Bhabha National Institute, Mumbai-400094, India*
**Corresponding author: debojyoti@barc.gov.in*

Planar dynamic loading experiments have been carried out on polycrystalline tungsten carbide in 63 mm bore Gas Gun facility to measure the Hugoniot data, Hugoniot Elastic Limit (HEL), dynamic yield strength and spall strength under high strain rates employing time resolved interferometery. The yield strength has been found to vary in the range 2.97-3.44 GPa for the peak shock pressure range of ~ 16-18 GPa. However, the spall strength observed to lie between 1.47 to 1.62 GPa, indicating sensitivity towards the applied peak shock pressure. Both the yield strength and spall strength are found to be significantly higher than their quasi-static loading counterparts.

**a0016**

**Cu at high pressure and high temperature: *Ab-initio* study**

Monika Rathod[1,a)], B. D. Sahoo[1] and K. D. Joshi[1,]
[1]*Applied Physics Division, Bhabha Atomic Research Centre, Mumbai, India 40008*
[2]*Homi Bhabha National Institute, Mumbai, India, 400094*
[a)] *Corresponding author: monikar@barc.gov.in*

The structural stability of copper has been analyzed under high pressure and high temperature, employing density functional theory and density functional perturbation theory based calculations. Enthalpy calculations as a function of pressure at 0 K, do not show any possibility of the face-centered cubic (FCC) to body-centered cubic (BCC) phase transition up to 400 GPa, consistent with previous theoretical studies. However, introduction of thermal effects within quasi harmonic approximations, suggest that upon heating above 2500 K at ~200 GPa, the FCC phase will transform to BCC phase. Further, lattice dynamical study revealed that the dynamical stability of FCC Cu persists from 0 GPa to 200 GPa, whereas the BCC phase emerges as dynamically stable structure from 20 GPa to 400GPa.The shock Hugoniot derived from theoretical calculations in conjunction with Rankine Hugoniot relation agrees well with the experimental data. Further, the P-T Hugoniot, indicates that the shock induced temperature rise could be one of the possible factors causing the experimentally observed FCC to BCC transition at ~180 GPa, under shock loading.

**a0017**

**Pressure Induced Amorphization in $Mg_2Si$**

[*]Ajinkya P. Khangal[1,2], Swastik Mondal[3], Ajay K. Mishra[1,2]
[1]*Homi Bhabha National Institute, Mumbai*
[2]*Bhabha Atomic Research Centre, Mumbai*
[3]*CSIR-Central Glass and Ceramic Research Institute, Kolkata*
[*]*Corresponding author: ajinkyakhangal@gmail.com*

The demand for abundant, non-toxic thermoelectric materials is steadily increasing due to the growing need for sustainable energy solutions. In this context, a new class of semiconducting compounds, metal silicides, has attracted significant interest recently.

Among these, magnesium silicide ($Mg_2Si$), which is an alkaline earth silicide is particularly promising candidate being non-toxic in nature, elemental abundance, and favorable thermoelectric properties. Our synchrotron based X-ray diffraction (XRD) measurements on this compound upto ~ 12 GPa, reveal a pressure induced amorphization beyond 8.1 GPa, which persists up to the highest pressure explored, in contrast to earlier studies which report pressure induced structural phase transitions. On decompression it retains its amorphous phase and does not revert back to its original phase, implying permanent amorphization and transition to a disordered state. Bulk modulus and its derivative were determined to be $K_0 = 38.95 \pm 8.68$ GPa and $K_0' = 8.78 \pm 1.72$ for cubic phase of $Mg_2Si$ using experimentally determined P-V data. This provides critical insights into the compressibility behaviour and structural evolution of $Mg_2Si$ under compression.

**a0018**

**Chemical and Physical Pressure Effects on Structural Properties of $RSn_4$-Type Topological Nodal-Line Semimetals**

Satheasuweatha M.N[1,2, a], Arumugam Sonachalam[2,3] and Boby Joseph[1, b]
[1]*Elettra-Sincrotrone Trieste S.C. p. A., S.S. 14, Km 163.5 in Area Science Park, Basovizza 34149, Italy.*
[2]*Center for High Pressure Research (CHPR), School of Physics, Bharathidasan University, Tiruchirappalli 620024, India*
[3]*Tamil Nadu Open University, Chennai 600 015, India*
**Email: a)sathyasweathamn05@gmail.com, b)boby.joseph@elettra.eu*

The $RSn_4$ (R= Au, Pt, and Pd) compounds have been reported to show exotic electronic properties due to their topological nodal line semi-metallic characteristics. These compounds share a common layered orthorhombic crystal structure but differ in their space group symmetries, which potentially influence their physical properties. Among them, $PtSn_4$ and $PdSn_4$ are isostructural compounds with the same Ccca space group. To explore the role of chemical pressure, we analyzed lattice parameters and compressibility through ambient and high-pressure structural data. The ambient unit cell volumes of $AuSn_4$ and $PdSn_4$ fall along with the negative pressure extrapolation of $PtSn_4$. Also, the bulk moduli of $PtSn_4$ and $PdSn_4$ indicate similar compressibility at low pressures. These observations suggest that $AuSn_4$ and $PdSn_4$ act as the negative chemical pressure equivalents to $PtSn_4$. Additionally, temperature-dependent resistivity measurements show that $AuSn_4$ exhibits a nonlinear trend, which may be due to increased electron scattering or lower symmetry, while $PtSn_4$ and $PdSn_4$ show nearly linear metallic behavior. $AuSn_4$ also shows superconductivity at 2.4 K, consistent with previous reports. These findings highlight how chemical pressure and symmetry govern the structural and electronic properties of $RSn_4$-type TNLS compounds.

**a0019**

**Structural Stability of α-$WP_2$ at High Pressure**

Arpita Aparajita A. N.[1,a)], Sanitha K.[1,3], Srihari V.[2] and Sanjay Kumar N. R.[1, 3]
[1]*High Pressure Studies Section, Condensed Matter Physics Division, Material Science Group, Indira Gandhi Centre for Atomic Research, Kalpakkam, Tamil Nadu, India, 603102.*
[2] *High Pressure & Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Mumbai, India, 40085*
[3]*Homi Bhabha National Institute, India*
[a)]*Corresponding author: arpita_an@igcar.gov.in*

The high-pressure behavior of α-$WP_2$ has been investigated up to 39 GPa, revealing that it remains structurally stable and is significantly less compressible than WP and β-$WP_2$. The compound exhibits anisotropic lattice compressibility, with the highest compressibility observed along the *b*-axis, and comparable compressibility along the *a*-and *c*-axis. This anisotropy is likely linked to the presence of covalent P–P bonds along the *a*-axis and metallic W–W interactions along the *b*-axis. The bulk modulus of α-$WP_2$ is estimated to be 278(20) GPa. Further investigation into the bonding nature within and between the $WP_5$ polyhedra is essential to fully understand the mechanical response of this material under pressure.

**a0021**

**Phonon-Mediated Phase Transitions in Scandium Under Pressure: A First-Principles Study**

Paras Patel [*]and Prafulla K. Jha
*Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, India-390002*
**Email: pparas727@gmail.com (Email of corresponding author)*

Understanding the mechanisms underlying structural phase transitions in rare-earth elements remains a central challenge in condensed matter physics and materials science. Scandium, although a transition metal, is often grouped with rare-earth elements due to its similar electronic and structural properties. Notably, scandium exhibits complex behaviour under high pressure. In this study, we perform a comprehensive investigation of scandium's structural evolution under pressure, focusing on its close-packed phases, hexagonal close-packed (*hcp*), face-centred cubic (*fcc*), and body- centred cubic (*bcc*) using state-of-the-art density functional theory (DFT) calculations. Our energetic analysis confirms that the *hcp* phase is stable under ambient conditions, while the *fcc* phase becomes energetically favourable at higher pressure above 40 GPa. Phonon dispersion calculations reveal the presence of soft acoustic modes in the *hcp* phase, which evolve into imaginary frequencies with increasing pressure, indicating dynamical instability. These results demonstrate that the structural phase transition in scandium could be primarily driven by vibrational instabilities rather than purely electronic effects.

**a0022**

**Temperature-Dependent Vibrational and Photoluminescence Studies on $ErNbO_4$**

Amit Tyagi[1,2*] & Alka B. Garg[1,2]
[1]*High Pressure and Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Mumbai, India 400085*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai, India 400094*
[*]*Corresponding author email: tyagiamit@barc.gov.in*
Rare-earth niobates ($R$NbO$_4$, where $R$ = rare-earth element) are recognized for their luminescence properties, making them attractive for optical applications like in photonics and optoelectronic applications. Among these, erbium orthoniobate (ErNbO$_4$) is distinguished by the efficient near-infrared and visible emissions of $Er^{3+}$ ions, governed by their unique crystal field environment. In this study, ErNbO$_4$ was synthesized using solid-state reaction method. Structural and vibrational analyses was conducted at ambient condition to ensure the formation of monoclinic fergusonite phase. Additionally, photoluminescence (PL) measurement was also carried out at ambient condition which shows intra-4f transitions of $Er^{3+}$ ions. High-temperature Raman and PL studies performed up to 600 °C, revealed the stability of ambient structure up to the maximum temperature. However, the PL intensity of the peak centered at ~660 nm (corresponding to the $^4F_{9/2}$ to $^4I_{15/2}$transition), is significantly enhanced at elevated temperatures.

**a0023**
**Implications Of Short-Range Structural Correlations Of $Pb^{2+}$ In Network-Forming Properties Of Lead-Borate Glasses: An EXAFS study**
Soumee Chakraborty[1,2, a)], Madhusmita Sahoo[3], Ashok Kumar Yadav[4], K. Prabakar[1,2] and Awadhesh Mani[1,2]
[1]*Condensed Matter Physics Division, Materials Science Group, Indira Gandhi Centre for Atomic Research, Kalpakkam, Tamil Nadu 603102, India.*
[2]*Homi Bhabha National Institute, Training School Complex, Anushaktinagar, Mumbai, Maharashtra 400094, India.*
[3]*Heavy Water Board Facilities, Talcher, Odisha 759106, India.*
[4]*Atomic and Molecular Physics Division, Physics Group, Bhabha Atomic Research Centre, Mumbai, Maharashtra 400085, India.*
**Email:soumee@igcar.gov.in*
Borate glasses exhibit unique behaviour known as borate anomaly where there is an inflation of properties around some intermediate composition of added network modifier. This is due to change in local co-ordination of the boron atom from $BO_3$ to $BO_4$, when the modifier is added to the system. In the present system of lead-borate glasses, PbO is the modifier oxide. As the local coordination and structure around the network forming cation, boron, is already well-reported, the atomic scale structure around the modifier cation, Pb, has been studied using x-ray absorption spectroscopy in this work. Herein, we report the Pb $L_3$-edge extended x-ray absorption fine structure (EXAFS) results to determine the local coordination environment of Pb ions in three $x$PbO: (1-$x$)$B_2O_3$ glasses with $x$ being 20, 40 and 80 mol%. A single shell fitting of EXAFS spectra of the glasses showed that lead is octahedrallyco-ordinated to oxygen when PbO concentration is 20% while it is tetrahedrallyco-ordinated when the concentration of PbO was 80%. The co-ordination number varied from 6.2 to 4.0 when PbO concentration varied from 20-80%. EXAFS studies helped in delineating the optimum concentration at which the local co-ordination change occurs and lead oxide manifests as a network former.

**a0024**
**Effect of Co-doping of Na and Sm on the Structural and Thermal Stability of $SrBi_4Ti_4O_{15}$/SBT Piezoelectric Ceramics**
Priyambada Nayak[1, a)], B. K. Satpathy[2]
[1]*Department of Physics, ITER, S'O'A deemed to be University,Khandagiri, Bhubaneswar, Odisha-751030, India*
[2]*School of Basic Science, Indian Institute of Technology, Bhubaneswar, Odisha-752050, India*
**[a)]Corresponding author: [a)]priyambada.pce@gmail.com*
$Sr_{1-x}Sm_xNa_xBi_4Ti_4O_{15}$ (x = 0.00, 0.05, 0.1, 0.15 and 0.2) bismuth layer structure ferroelectric ceramics (BLSFs) were prepared by simple solid-state reaction method. From the X-ray diffraction technique, it is depicted that all compositions show orthorhombic structure with $A2_1am$ space group. Dielectric study confirms that both dielectric permittivity and phase transition temperature ($T_C$) reduces with increasing amount of Na and Sm-content. Further lower value of tangent loss and thermal stability was achieved in the Na and Sm co-doped composition, which is mainly related to the oxygen vacancies mechanism. All the result indicated that the prepared modified ceramic is a suitable candidate for high temperature piezoelectric sensor application.

**a0025**
**Evolution of local structure in Nd, Fe modified Lead Titanate Ceramics**
ShiffaliMiddha[1], Sunil Kumar[1], Rachna Selvamani[2,*], Rekha Rao[2,3], and Anupinder Singh[1,*]
[1]*MultifunctionalMaterials Laboratory, Department of Physics, Guru Nanak Dev University, Punjab-143005, India*
[2]*Solid-State Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, India*
[3]*Homi Bhabha National Institute, Anushaktinagar, Mumbai-400085, India*
[*]*Email:anupinders@gmail.com*
Raman spectroscopy of $Nd_xPb_{1-x}Fe_xTi_{1-x}O_3$ ($x$=0.20,0.21,0.22,0.23,0.24) solid solutions was carried out at room temperature. All compositions exhibited characteristic Raman modes at 70 cm$^{-1}$, 200 cm$^{-1}$, 280 cm$^{-1}$, 550 cm$^{-1}$, and 700 cm$^{-1}$ in accordance with $C_{4v}^1$ (P4nma) space group, indicating the predominance of the tetragonal phase. Shift of E($TO_1$) soft mode from 88 to ~74 cm$^{-1}$ with Fe and Nd co-substitution, suggested a reduction in tetragonality and, consequently, a decrease in Curie temperature ($T_c$). Two new peaks at ~ 108 cm$^{-1}$ and 670 cm$^{-1}$ appeared for x ≥ 22. The intensity of these peaks increases with an increase in Nd and Fe

modification, indicating the emergence of an orthorhombic structure locally within the samples for x≥0.22. The findings reveal structural modifications in the ceramics and suggest further investigation into their structural properties.

**a0026**

**High Pressure study of ZIF-67 using IR spectroscopy and X-ray Diffraction**

Arkadev Roy,[1,3] Himal Bhatt,[1,3*] S. K. Sharma,[2] V. Srihari,[1] H. K. Poswal, [1,3] S. Vishwakarma[1] and T. Sakuntala,[1,3]
*High Pressure & Synchrotron Radiaiton Physics Division,[2]RCD, Bhabha Atomic Research Centre, Trombay, Mumbai, India 400085*
*[3]Homi Bhabha National Institute, Anushaktinagar, Mumbai, India 400094*
**Email:* hbhatt@barc.gov.in

We have presented a detailed high pressure study of ZIF-67 bulk powder, isostructural with widely discussed ZIF-8 compound, utilizing FTIR and synchrotron based X-ray diffraction measurements and employing Si oil as a non-penetrating PTM. An irreversible phase transition is observed upon compression to 8 GPa followed by a complete decompression. The framework structure collapses around 1 GPa and the material become amorphous. However, contrary to the crystal structure, chemical structure depicts significant durability as we have found the chemical structure to survive a compression of 12 GPa. FTIR spectra of the recovered sample resemble the IR profile near 1 GPa, indicating a partially reversible chemical transformation. This unusual behaviour of ZIF-67 may provide a new light into its' potential storage application.

**a0027**

**Structural and Vibrational properties of $Pb_2Bi(VxP1-x)O_6$ ($0.0 \leq x \leq 1.0$)**

Prasenjit Saha[a,b], SwathiJ[c], SwayamKesaria,b S. N. Achary[a,b],
*[a] Chemistry Division, Bhabha Atomic Research Centre, Mumbai, 400085, India*
*[b]HomiBhaba National Institute, Anushaktinagar, Mumbai. 400085, India.*
*[c]Loyola College Chennai Tamil Nadu 600 034*
**Email :[a] prasenjits@barc.gov.in*

Herein we report the structural & vibrational properties of compositions Bi3+ and Pb2+ containing compositions Pb2Bi(V1-xPx)O6 (0<x<1) prepared by solid state reaction. The compounds show closely related crystal structure with change in symmetry with change in nature and amounts of tetrahedral cations. A systemic decrease in molar volume with increasing PO4 content is observed and that has been attributed to smaller volume of PO4 units. Besides, it is suggested that the increase in symmetry along the composition with increasing PO4 content might be related to the free and ease orientation of PO4 groups in the lattice. Local structure studied from Raman spectroscopy indicated all the sample have closely similar local environment.

**a0028**

**Low Temperature Phase Transition Study of $WO_3$ using Raman Spectroscopy**

S.R Vishwakarma[1,] Himal Bhatt[1, 2,a)], Harsha Kumawat[1,2], T. Sakuntala[1,2]
*[1]High Pressure & Synchrotron Radiation Division, Bhabha Atomic research center, Trombay, Mumbai, India-400085. [2]Homi Bhabha National Institute, Anushaktinagar, Mumbai, India 400094.*
*[a)]Email: hbhatt@barc.gov.in*

In this work we have studied temperature induced phase transitions in tungsten oxide ($WO_3$) using Raman spectroscopy from room temperature to low temperature down to -180°C. The compound is used in several applications, including those involving temperature treatments. We used the powder form of sample without any pressure or other thermodynamic treatments. The compound exists in monoclinic (I) structure at room temperature and systematically transforms to triclinic and monoclinic (II) structures upon cooling. We specifically probed the reversibility of these phase transitions during cooling and heating temperature cycles by studying the behavior of fingerprint and lattice Raman modes. Clear deviations were observed in the spectral profile between room temperature and after undergoing the temperature cycles. We show here that the peak positions as well as intensities of characteristic Raman modes used as markers to show changes under thermodynamic variations, depict a hysteresis behavior, highlighting the fact that the room temperature phase cannot be completely retrieved upon temperature treatment.

**a0030**

**Atomistic study of shock induced phase transformations and Hugoniot elastic limit (HEL) in single crystal copper**

B. D. Sahoo[1,a)], K. D. Joshi[1,2]
[1]*Applied Physics Division, Bhabha Atomic Research Centre, Mumbai, India 400085*
[2] *Homi Bhabha National Institute, Mumbai, India, 400094*
*[a)] Corresponding author: bdsahoo@barc.gov.in*

Large-scale nonequilibrium Molecular Dynamics (NEMD) Simulations with a realistic embedded atom potential have been used to investigate the behavior of bulk single crystal of Cu subjected to shock loading in different crystal orientation with piston velocities ranging from 250 m/s to 3000 m/s. Our NEMD simulation reports the FCC–BCC phase transition in Cu single crystal to occur at pressures ≥126 GPa, when loaded along <100> direction and at pressures ≥185 GPa upon loading along <110> direction. The same transition is reported experimentally to happen at 180 GPa in polycrystalline sample. Also determined, is the Hugoniot elastic limit (HEL) and its dependence on associated physical parameters (length and time scale).

**a0031**

**Raman Spectroscopy Insights into Short-Range Ordering and Abrupt Line-Shape Evolution During Laser-Induced Crystallization of Amorphous Germanium**

Sharmistha Singh[1] and Rajesh Kumar[1,*]

*[1]Materials and Device Lab, Department of Physics, Indian Institute of Technology Indore, Simrol-453552, India*

**Email: rajeshkumar@iiti.ac.in*

The microscopic properties of materials can be understood through Raman spectroscopy, enabling their optimization for various technological applications. This study examines the impact of laser-induced heating on amorphous germanium (a-Ge), analyzed through Raman scattering. The broad Raman spectrum centered at 269 $cm^{-1}$, from as-deposited a-Ge film, is replaced by an asymmetric Raman line shape centered at 298 $cm^{-1}$ on crystallization. The experimentally observed nano-crystallization of amorphous thin films has been quantitatively assessed using the established phonon confinement model (PCM) and the modified phonon confinement model (MPCM) and further validated using the bond polarization model (BPM). The integration of existing theoretical frameworks and the proposed empirical model effectively characterizes the amorphous-to-nano-crystalline phase transition in germanium thin films, enabling precise quantification of short-range order and nano-crystallite dimensions in both amorphous and nano-crystalline germanium.

**a0032**

**Electronic, Magnetic And Thermodynamic Properties Of High-Spin Metallic $Ce_4Ni_3O_8$: A First-Principles Study**

Surendra Singh Senger[1 a)] and Dinesh C. Gupta[2]

*[1,2]Condensed Matter Theory Group, School of Studies in Physics, Jiwaji University, Gwalior – 474011 (M.P.), India*

*[a)] Corresponding author: sengar.physics@gmail.com[1], sosfizix@gmail.com[2]*

We report a first-principles investigation of the structural, electronic, magnetic properties of layered nickelate $Ce_4Ni_3O_8$. Density functional theory (DFT) calculations were carried out within GGA and the modified Becke–Johnson potential to treat strong electronic correlations. $Ce_4Ni_3O_8$ stabilizes in a ferromagnetic metallic ground state. The electronic structure reveals dominant Ni-3d and O-2p states near the Fermi level, while Ce-4f orbitals contribute to localized magnetism. Thermodynamic results indicate stable phonon behaviour and favourable heat capacity trends.

# b) Soft matter including biological systems

**b0001**

**The Physics behind the Antimicrobial Action of the Aurein Peptide**

V. K. Sharma[1*] and S. Qian[2]
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai, India 400085*
[2]*Homi Bhabha National Institute, Mumbai, India 400 094*
[3]*Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830, United States.*
**Email:sharmavk@barc.gov.in (Email of corresponding author)*

Antimicrobial peptides (AMPs) are front-line candidates against drug-resistant bacteria, yet their therapeutic promise demands precise selectivity for bacterial over mammalian membranes, a property dictated by lipid composition. Using neutron membrane diffraction and spin-echo spectroscopy, we show that aurein 1.2 softens zwitterionic DMPC bilayers (model mammalian membranes) by thinning the membrane and enhancing bending fluctuations, with a monotonic decrease in bending modulus up to P/L = 4 %. Strikingly, unlike its stiffening at high P/L in mixed zwitterionic–anionic membranes (bacterial models), no stiffening emerges here. These results expose a pronounced composition-dependent switch in aurein's interaction mechanism, offering molecular insight into AMP selectivity.

**b0002**

**Dynamics of Choline Chloride based Deep Eutectic Solvents: Neutron Scattering Study**

Rinesh T.[1,2], H. Srinivasan[1,2], V.K. Sharma[1,2] and S. Mitra[1,2]*
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai, India - 400085*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*
**Email:smitra@barc.gov.in*

In this study, we investigate the microscopic diffusion dynamics of choline chloride (ChCl) based deep eutectic solvents (DESs) to elucidate the influence of hydrogen bond donor (HBD) identity on the mobility of cholinium ions. The DES systems examined include ethaline, glyceline, and reline, comprising ChCl mixed with ethylene glycol, glycerol, and urea, respectively, in a 1:2 molar ratio. Quasielastic neutron scattering experiments was used to probe the self-diffusion of cholinium ions at molecular length and time scales. The dynamics were modelled as a combination of jump diffusion of the molecular center of mass and localized translation within transient hydrogen-bond cages. Among the three systems, ethaline consistently exhibited the highest cholinium self-diffusion coefficients across all investigated temperatures, attributed to shorter residence times and more frequent molecular jumps. In contrast, reline displayed longer residence times with significantly larger jump length, leading to a temperature-dependent dynamical crossover: While reline and glyceline exhibited comparable diffusivities at low temperatures, reline surpassed glyceline above 330 K. These findings highlight the crucial role of HBD identity in modulating microscopic diffusion and provide valuable molecular-level insights for the rational design of DESs for targeted applications.

**b0003**

**Encapsulation of Nano Cellulose within Nano-porous Silica Shell using Evaporation Induced Assembly**

Ankur Saha[1,2], Debasis Sen[1,2, a)],N Vigneshwaran[3],A K Bharimalla[3], Avik Das[1] and Jitendra Bahadur[1,2]
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai-400085,India.*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai-400094, India.*
[3]*ICAR-Central Institute for Research on Cotton Technology, Mumbai 400019, India*
[a)]*Email: debasis@barc.gov.in*

Encapsulation of bio-derived nanomaterials within inorganic matrices offers a promising route to enhance their functional stability and applicability. In this work, we demonstrate a facile, one-step spray drying method to encapsulate cellulose nanocrystals (CNCs) in the interstices ofsilica nanoparticles. CNCs, widely used for high aspect ratio, large area of charged surfaces, were mixed with colloidal nano-silica dispersion and atomized into hot air. The fast-drying process generated concentration gradients and capillary flows, driving different movements of CNCs and silica particles based on their diffusivity and interactions. Morphological characterization confirmed that the CNCs get trapped within the nano-porous silica shell, forming a core-shell structure. This method offers a scalable and energy-efficient approach to fabricate bio-inorganic hybrid materials with potential applications in drug delivery, nanocomposites, and sustainable coatings.

**b0004**

**Pacman Particles at Play: Hybrid Colloidal Systems for Reconfigurable Microstructured Materials**

Indira Barros and Indrani Chakraborty
*Department of Physics, Birla Institute of Technology and Science, Pilani-K K Birla Goa Campus, Zuarinagar, Goa 403726, India*
**Email:indranic@goa.bits-pilani.ac.in*

We investigate the field-directed assembly of patchy colloidal particles composed of magnetic hematite cubes encapsulated in TPM shells. These "Pacman-like" particles exhibit specific interactions via their magnetic patch, enabling tunable structures under external fields. A magnetic field drives patch-to-patch interactions, while an AC electric field induces stacking and spreading. By using this multi-field combination and by varying field parameters, such as frequency and amplitude we achieve programmable transitions between distinct assembly modes. Our work offers a versatile platform for designing reconfigurable colloidal architectures with potential applications in micro-robotics and smart materials.

**b0005**

**Frank Elastic Constants for 2D Nematic Liquid Crystals**

Peerizah Manav Singh and Debabrata Deb

*Department of Physics and Materials Science, Thapar Institute of Engineering and Technology, Patiala-147004, Punjab, India*

*Email: peerizah9999@gmail.com, debabrata.deb@thapar.edu*

We present a computational study of the Frank elastic constants, namely splay $K_1$ and bend $K_3$ for a nematic liquid crystalline system composed of 2D anisotropic particles interacting via the Gay-Berne (GB) potential having parameters (3,5,2,1). Using large-scale molecular dynamics simulations, we extract the elastic constants through the molecular orientation fluctuations based approach. It has been observed that the elastic anisotropy, characterized by the ratio $K_3/K_1$, increases with the particle's density and decreases with temperature.

**b0006**

**Chiral Active Gyrator: Diffusive Dynamics**

Deion Santhosh and Mamata Sahoo

*Department of Physics, University of Kerala, Kariavattom, Thiruvananthapuram-695581, India.*

**Email: mamata@keralauniversity.ac.in*

We theoretically explore the diffusive dynamics of an inertial chiral active Ornstein-Uhlenbeck particle in a two dimensional anisotropic harmonic potential and immersed in a viscous medium. The system is driven by two different thermal baths along the two orthogonal directions of the potential. The motion is governed by underdamped Langevin equations with inertia and constant active torque. In the steady state, the anisotropy in diffusion in the $x$ and $y$ directions arises even in the absence of a temperature gradient, purely due to chirality. For a fixed temperature gradient, the anisotropy in both $x$ and $y$ directions exhibits a non-monotonic dependence on chirality: it first increases, shows a maximum, and then decreases. Moreover, for a very high chirality strength, the system recovers the isotropy in diffusion in both $x$ and $y$ directions even in the absence of a temperature gradient.

**b0008**

**Tuning Sol-Gel Transitions in BSA Protein Systems via Nanoparticle Interactions**

Soumya[1, 2], Sugam Kumar[1, 2, a)] and V. K. Aswal[1, 2]

*[1]Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085 India*

*[2]Homi Bhabha National Institute, Mumbai 400094, India.*

*[a)] Corresponding author: sugam@barc.gov.in*

Sol–gel transitions in protein systems play a vital role in designing functional biomaterials with tunable properties. In this study, we investigate thermal gelation of bovine serum albumin (BSA) at pH ~5 and demonstrate how silica nanoparticles influence this process. Heating causes BSA to unfold and aggregate via hydrophobic interactions, forming opaque gels. However, introducing anionic silica nanoparticles delays gelation and enhances optical transparency. Dynamic light scattering reveals slower growth in size, while zeta potential measurements indicate increased surface charge, promoting electrostatic repulsion. At higher nanoparticle concentrations, gelation is completely suppressed. The resulting hydrogels are softer and more transparent. This strategy enables controlled tuning of gel properties, making these systems suitable for applications in biosensing, diagnostics, and soft materials engineering.

**b0009**

**Biomicrorheology via Particle-tracking in *yeast* under organelle mutations**

Sruthi Kaladharan[1], Chhaya Kispotta[2], Krishnaveni Mishra[3], Sharath Ananthamurthy[4]

*[1,4]School of Physics, University Of Hyderabad, Telangana-500046*

*[2,3]Dept. Of Biochemistry, School Of Life Sciences, University Of Hyderabad, Telangana-500046*

** Corresponding author:* sasp@uohyd.ac.in

This study investigates the impact of endoplasmic reticulum (ER) mutations on the biophysical properties of the cytoplasm in *Saccharomyces cerevisiae*. Using particle- tracking microrheology, we quantify how perturbations in ER morphology—specifically through deletions of *RTN1* and *YOP1* —alter intracellular viscosity and viscoelastic- ity. This integrated approach provides insights into how organelle structure influences mesoscale transport and mechanical behavior in living cells.

**b0010**

**Coarse-Grained Dean's Equation for Active Brownian Particles with Position-Dependent Dissipation**

Sunil Kumar Yadav

*P. G. Department of Physics, Veer Kunwar Singh University, Ara, Bihar 802301, India*

**Email:*sunil1507@yahoo.com

Starting with the microscopic Langevin equation for a single active Brownian particle, which contains an active noise term, a macroscopic equation for mass density is obtained. The overdamped limit is taken, and the time dependence of momentum is ignored. Frictional drag is taken to be position-dependent. Active noise in the microscopic equation drives the system in a non-equilibrium state. An exact balance equation for the microscopic mass density is obtained. The microscopic equation, having

position coordinates only, is averaged over the local equilibrium ensemble. This obtains the stochastic time evolution equation for macroscopic mass density. This equation contains multiplicative noise and additional terms that are absent in the Dean's equation for passive Brownian particles.

**b0011**

**Controlling Modulation of Interactions during Re-entrant Phase Behavior in Nanoparticle-Polymer System**

Sushma[1,2,*], Sugam Kumar[1,2] and Vinod K. Aswal[1, 2]
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085 India*
[2]*Homi Bhabha National Institute, Mumbai 400094, India.*
**Email:sushmalad@barc.gov.in*

Nanoparticle–polymer systems show versatile phase behavior, originating from the nanoscale properties of nanoparticles and tunable chemistry of polymers, providing excellent platforms for designing soft materials with functional properties. The dispersions of anionic silica nanoparticles in non-ionic polyethylene glycol (PEG) solutions exhibit a distinctive re-entrant phase behavior, where system undergoes a transition stable phase to aggregated phase and then retun back to stable phase with increasing polymer concentration. This behavior is marked by a rise and subsequent decline in both hydrodynamic size and viscosity, indicating initial aggregation followed by re-stabilization. We show that the boundaries of these phases can be finely tuned by varying the nanoparticle concentration and ionic strength in the system. These findings highlight the role of polymer-mediated interactions in governing colloidal stability and demonstrate a controllable strategy to engineer responsive nanoparticle–polymer systems.

**b0012**

**Positron Annihilation Lifetime Spectroscopic (PALS) Study on Crystalline and Amorphous Silica Nano-pores under High $CO_2$ Gas Pressure**

Shapath Bhandari[1] and Dhanadeep Dutta[1, 2, *]
[1]*Radiochemistry Division, Bhabha Atomic Research centre, Trombay, Mumbai-400 085*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai-400 094*
[*]*Corresponding author: deep@barc.gov.in*

Positron annihilation lifetime spectroscopy (PALS) has been utilized to observe the distinction of pore-filling mechanism of $CO_2$ in SBA-15 and silica nanaopores. The SBA-15 has well-ordered hexagonal mesopores connected through smaller micropores at the mesopore walls, whereas amorphous silica nanopores are oriented in disordered manner. The PALS result revealed that despite rigid pore structure of SBA-15, spin-triplet *ortho*-positronium (*o*-Ps) lifetime corresponding to micropores showed an increasing trend upto 75 psi pressure and then decreased at higher $CO_2$ pressure, whereas in disordered silica micropores no such increase in *o*-Ps lifetime has been observed at lower pressure. The increase in *o*-Ps lifetime (or decrease in *o*-Ps annihilation rate) in ordered micro-pores at low $CO_2$ pressure may correspond to the reduction in *o*-Ps diffusion from micropores to the mesopores in ordered SBA-15 pore structure, where as in disordered micropores, *o*-Ps did not show any diffusive motion from micro to the mesopores. An extrapolation of straight line fitting of *o*-Ps annihilation rate to zero $CO_2$ pressure may give true *pick-off* annihilation rate inside the micropores of SBA-15 in vacuum. Above ~400 psi $CO_2$ pressure, *o*-Ps annihilation rate inside micropore was seen to be saturated, probably due to liquification of $CO_2$ inside the micropores. However, the *o*-Ps annihilation rate in mesopores of both SBA-15 and silica under $CO_2$ pressure showed similar increasing trend like that of bulk $CO_2$ gas.

**b0014**

**Water uptake and release kinetics of Laponite-Acrylamide hybrid hydrogels**

Tanay Saha, and ParameshGadige[*]
*Department of Physics, Sri Sathya Sai Institute of Higher Learning, PrashanthiNilayam Campus, Puttaparthi, 515134, Andhra Pradesh, India.*
**Email:gadigeparamesh@sssihl.edu.in*

In this study, hybrid hydrogel composed of Laponite (Lap), Acrylic Acid (AA), and Acrylamide (AAm) with no additional cross-linkersis synthesized to investigate its water uptake and release kinetics as well as swelling characteristics. Lap, a synthetic nanoclay of layered silicate is incorporated into the poly (AA-AAm)network via free-radical polymerization to study its effect on the hydrogel's swelling characteristics at neutral pH.The water uptake and swelling behavior is evaluated by measuring the weight and dimensions of the samples as a function time by immersing in water.Similarly,water release (deswelling) kinetics are studied during the drying process at room temperature by measuring the weight, which has provided insights into its potential for controlled release and smart material applications. The incorporation of Lap at intermediate low concertation has shown high water uptake capacity and deswelling, which is attributed to the cross-linking of the charged Lap nano particles with the AA-AAm polymer network.

**b0015**

**Non-Markovian Gyrator**

Soorya Sunil[1], Adersh Fernandez[1] and Mamata Sahoo[1, a)]
[1]*Department of Physics, University of Kerala, Kariavattom, Thiruvananthapuram-695581,India.*
**Email: mamata@keralauniversity.ac.in*

We investigate the two-dimensional motion of a Brownian particle confined in an asymmetric harmonic potential and coupled to two thermal baths maintained at different temperatures. Such a system exhibits gyration due to the combined effects of temperature gradient and potential asymmetry. We examine how the gyrating behavior is affected when the system is immersed in a non-Markovian environment characterized by a finite memory timescale. We have exactly calculated the angular velocity and observe that memory introduces a non-monotonic dependence of angular velocity on the potential asymmetry. Moreover, the peak in angular velocity shifts toward lower asymmetry values as the memory timescale increases, indicating that the optimal asymmetry required for maximum rotation can be tuned by varying the persistent duration of memory. Further, we observe a self-inversion in the rotational motion by tuning the temperature gradient.

**b0016**

**Low-Threshold, Fast-Response Carbon Nanotube–Liquid Crystal Hybrid Systems with Tunable Optical and Dielectric Properties**

Suraj Joshi*and Rajiv Manohar
*Liquid Crystal Research Laboratory, Department of Physics, University of Lucknow, Lucknow, U.P., India 226007.*
**Email:007surajjoshi@gmail.com*

We report on the development of low-threshold, fast-response hybrid systems composed of single-walled carbon nanotube (SWCNT) doped nematic liquid crystal (NLC) ZLI 2976 with tunable optical and dielectric properties. The SWCNT–NLC composites demonstrate a significant reduction in threshold voltage (up to 82.4%) and switching time (up to 62.8%) as a function of nanotube concentration, enabling efficient low-power optical switching. UV–Vis absorption spectra reveal a redshift and narrowing of peaks alongside an increased optical bandgap, indicating enhanced molecular ordering and electronic transitions. Dielectric measurements show a pronounced permittivity and loss variation with frequency, while conductivity analysis identifies a percolation threshold corresponding to the formation of conductive networks within the composite. These findings highlight the potential of SWCNT–NLC hybrids as adaptable materials for advanced photonic devices in quantum and neuromorphic computing applications.

**b0017**

**Impact of Roughness on the Transport Coherence of an Overdamped Rocking Ratchet**

Prathyusha S Nair and Ronald Benjamin*
*Department of Physics, Cochin University of Science and Technology, Cochin, Ernakulam, Kerala - 682022*
**Email: rbenjamin.phys@gmail.com*

In this work, we investigate the transport coherence of an overdamped Brownian particle in a periodic rough potential driven by a time-dependent force in the presence of a thermal bath. We delve into the impact of roughness on the transport by analysing several transport properties such as the current, effective diffusion coefficient, and Peclet number as a function of the amplitude of the rough potential. We find that roughness improves particle current and coherency at low temperatures and optimal values of the amplitude and spatial frequency of the rough potential.

**b0018**

**Electric Field-Assisted Morphogenesis in Protein Crystallization**

*Debes Ray[1,2,*], M. Madani[3], J.K.G. Dhont[2,3], F. Platten[2,3] and K. Kang[2,3]*
*[1]Solid State Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400085, India*
*[2]Institute of Biological Information Processing IBI-4, ForschungszentrumJülich, 52428, Germany*
*[3]Faculty of Mathematics and Natural Sciences, Heinrich Heine University Düsseldorf, 40225 Düsseldorf, Germany*
**Email: debes@barc.gov.in*

A weak alternating current electric field significantly influences the position of the crystallization boundary, the liquid–liquid phase separation (LLPS) line, and the crystallization kinetics in lysozyme solutions containing sodium thiocyanate (NaSCN). In this study, we investigated how such an electric field affects the microscopic morphology of lysozyme crystals as they form from a supersaturated solution. A diverse range of distinct crystal shapes was observed, including single- and multi-armed structures, flower-like forms, whiskers, and sea urchin-like crystals. These crystal morphologies vary notably with changes in protein and salt concentrations, and the electric field markedly modifies the morphology-state diagram across the protein–salt concentration space. This modification is likely driven by the electric field's influence on protein–protein interactions. We propose that this effect arises from enhanced adsorption of $SCN^-$ ions onto the lysozyme surface under the electric field, which ultimately governs the observed crystallization behavior. These results provide valuable insights into how electric fields can be harnessed to control crystal growth and morphology in protein systems.

**b0019**

**Transport Coherence of a Fluctuating force Brownian ratchet**

Arjun S R and Ronald Benjamin*
*Department of Physics, Cochin University of Science and Technology, Kochi, Kerala, India-682022*
**Email:rbenjamin.phys@gmail.com*

The transport coherence of a Brownian particle driven by dichotomous perturbations, also known as the Fluctuating force ratchet or the run and tumble ratchet, is studied via numerical simulations of the overdamped Langevin equation. We analyze the particle

current, effective diffusion coefficient, and the Peclet number ($Pe$), which characterizes the transport coherence, by carrying out simulations to explore the effects of the magnitude of the fluctuating force ($v_0$), the temperature and the switching rate $\tau$ of the fluctuating force, in achieving regular transport. The average current shows a non-monotonic dependence on the fluctuating force, while the diffusivity rises monotonically with increasing $v_0$, suppressing the transport coherence. The effective diffusion coefficient increases, and the Peclet number, in general, decreases with increasing temperature. However, at low values of $v_0$, there exists an optimal temperature at which$Pe$ is maximized, though the transport coherence is poor. In the non-adiabatic regime and at low temperatures, $Pe$ is just above the threshold at which transport is considered to be coherent.

**b0020**

**Structural Invariance of Hyper-crystallizable PF1765 from *Pyrococcusfuriosus* Across Diverse Conditions**

Beena Yadav and Ravindra D. Makde*
*Department of Bioscience and Biomedical Engineering, Indian Institute of Technology Indore, 453552, Madhya Pradesh, India.*
*Beamline Development and Application Section, Bhabha Atomic Research Centre, Mumbai 400085, Maharashtra, India.*
**Email:ravimakde@rrcat.gov.in*

Understanding how crystallization conditions affect protein structure remains essential for interpreting X-ray crystallographic data. While prior studies have shown minimal structural variation among proteins crystallized under diverse conditions, most lacked control over batch-to-batch variation. Here, we systematically examine the structural impact of crystallization conditions using PF1765 from *Pyrococcusfuriosus*, a hyper-crystallizable and evolutionarily conserved protein. Using a single protein batch, we determined nine high-resolution structures (1.1–1.6 Å), from chemically distinct conditions, and compared with a previously deposited structure (PDB: 9UNT), yielding ten structures across two space groups: $P2_12_12_1$ and $P4_12_12$. Despite variations in pH, salts, and precipitants, all structures exhibit strong backbone conservation (Cα RMSD: 0.10–0.22 Å). Structures within the same space group were nearly indistinguishable, while modest, reproducible rotameric differences were observed between space groups. These findings demonstrate that crystallization environment and lattice symmetry primarily affect side-chain conformations, not global fold, and establish PF1765 as a robust model for assessing lattice-induced microheterogeneity.

**b0021**

**Tuning Fluctuation-Induced Casimir Forces in Porous Colloidal Systems Using Embedded Metal Nanoparticles**

Sarath Kumar R. M., Deepak K. Gupta [a)], K. Prabakar and A. Mani
*Condensed Matter Physics Division, Materials Science Group, Indira Gandhi Centre for Atomic Research, A CI of Homi Bhabha National Institute, Kalpakkam 603102, Tamilnadu, India*
**Email:dkg@igcar.gov.in*

Casimir force is a direct macroscopic manifestation of quantum field theory and plays an important role in nanoscience and nanotechnology owing to their piconewton strength, short range and tunability with surrounding temperature and shape of the objects involved. This study explores the enhancement of Casimir forces in porous polystyrene microspheres via incorporation of gold nanoparticles (AuNPs). Using the Boundary Element Method we simulated interactions between (i) isolated AuNPs, (ii) porous polystyrene spheres and (iii) hybrid structures with embedded AuNPs. Porous polystyrene spheres increased Casimir forces from sub-piconewton to several piconewtons, and incorporation of AuNPs inside enhanced the interaction range beyond 100 nm. While isolated AuNPs show negligible forces beyond this range, hybrids maintain measurable attraction due to the composite's collective electromagnetic response. The results highlight nanoparticle–polymer hybrids as a tunable platform for controlling fluctuation-induced forces, offering pathways for designing responsive colloidal assemblies and controlling nanoscale interactions in soft matter systems.

**b0022**

**Organo-Capped Gold Nanoparticle-Reinforced Starch-Based Nanocomposite Films with Enhanced Flexibility**

Nikesh Kumar [1, 2 *],SaiyadAkhirul Ali [1, 2] , SarathiKundu[1, 2]
*[1] Soft Nano Laboratory, Physical Sciences Division, Institute of Advanced Study in Science and Technology (IASST), Vigyan Path, PaschimBoragaon, Garchuk, Guwahati, Assam 781035, India*
*[2] Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002, India*
**Email:nikeshk01@gmail.com*

Starch, a biodegradable biopolymer, is valued for sustainable material development but limited by poor mechanical and thermal properties. To address this, cross-linked starch–gold St(c)-AuNanocomposite films were prepared by incorporating gold nanoparticles (AuNPs) into the starch matrix. Spectroscopic and microscopic analyses confirmed AuNP formation, St(c)-AuNP interactions, and structural changes. UV–visible spectroscopy revealed characteristic AuNP absorption peaks influencing mechanical performance, while TEM and SEM showed nanoparticle formation and uniform dispersion. Thermal (TGA) analysis indicated higher degradation temperatures, and stress–strain tests showed improved flexibility, with elongation up to 129%. These enhancements suggest St(c)-Au films as promising biodegradable packaging and coating materials.

**b0023**

**Effect of Macromolecular Crowding on Linear and Ring Polymer**

Rahul Bag and Surya K. Ghosh*
*Department of Physics, National Institute of Technology, Warangal, 506004, India*

*Email:skghosh@nitw.ac.in
Biopolymers such as DNA, RNA, FtsZ etc, can exist in both linear and ring conformations, each exhibiting distinct dynamical and structural behaviors in crowded cellular environments. Using extensive Langevin dynamics simulations, we compare the dynamics of linear and ring polymers with varying flexibility under different crowding conditions. While the mean-squared displacement (MSD) shows a similar dependence on packing fraction and flexibility for both topologies, the radius of gyration of ring polymers is significantly more sensitive to changes in crowding and flexibility with respect to linear polymers.

**b0024**

**Dielectric and Electro-Optical Study of a Biphenyl benzoate based Ferroelectric Liquid Crystal**

Himangshu Roy[1],Asim Debnath[1],Debarghya Goswami[2]and Sripada Haldar[1]
[1]*Department of Physics, North Bengal University, Siliguri,734013, India*
[2]*Department of Physics, St. Joseph's College, Northpoint, Darjeeling,734104, India*
*Email: nbushaldar@nbu.ac.in*

Newly synthesized biphenyl benzoate based smectic ferroelectric liquid crystal (FLC), (S)-(+)-4′-(3-pentanoyloxyeth-1-oxy)biphenyl-4-yl-4-(1-methylheptyloxy)benzoate (code name 4H2R), has been characterized by optical polarizing microscopy, dielectric spectroscopy and electro- optic investigations. Optical polarizing microscopy study reveals that it exhibit ferroelectric SmC* and cholesteric N* phase. In dielectric study Gold stone mode relaxation has been observed in the SmC* phase. Spontaneous polarization ($P_S$), switching time ($\tau$), and rotational viscosity ($\gamma_\varphi$) of the SmC* phase, have also been measured as function of temperature. $P_S$, $\tau$, and $\gamma_\varphi$ are found to be in the range of 88-165nC/cm$^2$, 1.11-1.44ms and 1.72- 4.16 N-s/m$^2$ respectively.

**b0027**

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

Sandeep Kushawah and Prasanth P. Jose
*School of Physical Sciences, IIT Mandi, Mandi-175005, H.P., India.*
*Email:prasanth@iitmandi.ac.in*

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.

**b0028**

**Effect of Ti Doping on Bioactivity of Borate Bioglasses**

RamuGangu, Tanay Saha, Tejash Kumar and Paramesh Gadige*
*Department of Physics, Sri Sathya Sai Institute of Higher Learning, PrashanthiNilayam Campus, Puttaparthi, 515134, Andhra Pradesh, India.*
**Email: gadigeparamesh@sssihl.edu.in*

Numerous bioactive glass compositions have been proposed for cutting-edge biomedical applications, such as soft tissue engineering, drug delivery, bone and dental repair. In this study, the effect of Ti doping on bioactivity of the biodegradable borate bioglass (1393-B3)is investigated, obtained by conventional melt-quenching process. Ti modified glasses including the parent 1393-B3 glass have shown in-vitro bioactivity in simulated body fluid (SBF). The glasses confirmed the formation of the hydroxyapatite (HA) phase over the glass surface. The bioactivity mechanism is attributed to the set of dissolution –precipitation reactions similar to the 45S5 silicate bioglass. Melt-derived bioactive glasses with the borate1393-B3 configurations degraded rapidly and converted to a calcium phosphate product when immersed in SBF. The $PO_4^{3-}$ groups from the solution respond to $Ca^{2+}$ situated on the glass surface, prompting the nucleation of HA. Where, the incorporation of Ti into the borate network enhanced the bioactivity due to its intrinsic bioactive characteristics.

**b0029**

**Elastic Properties of Erbium Doped Lithium Zinc Phosphate Glasses**

*Shwetha M[1, a)] and B Eraiah[2]*
[1]*Government Science College (Autonomous), Hassan- 573201, Karnataka, India*
[2]*Department of Physics, Bangalore University, Bengaluru-560056, Karnataka, India*
**Email:shwetha.sep89@gmail.com*

Erbium-doped phosphate glasses with the composition x mol% $Er_2O_3$ – 40 mol% $P_2O_5$ – 45 mol% ZnO – (15–x) mol% $Li_2O$ (x = 0 to 2 mol%) were synthesized via melt quenching and labeled ErP0 to ErP20. Structural, morphological, and mechanical characterizations were carried out using X-ray diffraction (XRD), scanning electron microscopy (SEM) with energy-dispersive spectroscopy (EDS), and theoretical modeling based on Makishima–Mackenzie theory. XRD patterns revealed broad humps, confirming the amorphous nature of all samples. SEM images exhibited smooth surfaces with no visible crystallites, and EDS spectra confirmed the presence of P, O, Zn, and Er elements. Mechanical properties such as Young's modulus, bulk modulus, shear modulus, Poisson's ratio, hardness, and fractal bond connectivity were calculated and analyzed. A slight decrease in modulus values

with increasing $Er_2O_3$ content is attributed to reduced packing density. The Poisson's ratio (~0.1151–0.1163) suggests a high cross-link density and fractal bond connectivity ($d \approx 2$) indicates a 2D layered structure. These findings confirm that the prepared glasses maintain good mechanical stability and possess structural characteristics favorable for photonic and optoelectronic applications.

**b0030**

**Effect of dimerization in relaxation dynamics in Supercooled Binary Mixture**

Devansu Chakraborty[1,a] and Prasanth P. Jose,[1,b]
[1] *School of Physical Science, Indian Institute of Technology Mandi, Kamand, Mandi 175005, India*
[(a)]*d21081@students.iitmandi.ac.in*
[(b)]*Corresponding author: prasanth@iitmandi.ac.in*

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

**b0031**

**Pressure, concentration and temperature dependent dynamical investigation of relaxations associated with hydrogen bonding in 1-propanol**

Anand K. Tiwari[1,2], Markus Appel[1], Bela farago[1], Miguel A. Gonzalez[1],Bo Jakobsen[2],Kristine Niss[2]
[1]*Institut Max von Laue - Paul Langevin (ILL), France*
[2]*Glass &Time, Department of Science and Environment (INM), Roskilde University, Denmark*
**Email: tiwari@ill.fr*

Hydrogen bonds are ubiquitous in nature and play a central role in determining the microscopic dynamics of liquids. While water remains the most important hydrogen-bonded liquid, its peculiar behaviour and supercooling challenges motivate the study of simpler systems, such as mono-hydroxy alcohols, where hydrogen-bond dynamics are better separated from structural relaxation. Dielectric spectroscopy has shown that mono-hydroxy alcohols exhibit a dominant slow Debye relaxation, slower than the α-relaxation, and growing evidence suggests that poly-alcohols display a similar, though more merged, separation of processes. In this work, we investigate the relaxation dynamics of liquid 1-propanol and its 10% glycerol mixture above the glass transition using quasi-elastic and inelastic neutron scattering (IN16B backscattering, wide-angle spin-echo, and IN5 time-of-flight) combined with dielectric spectroscopy. High-pressure measurements up to 3 kbar reveal that the slowest relaxation process shifts by nearly two orders of magnitude, whereas faster processes are largely unaffected, enabling the possibility of their complete separation. The effect of increasing hydrogen-bond concentration is probed by adding glycerol, which enhances the slowest component of the signal. Selective deuteration demonstrates that this slow dynamic originates from intermolecular hydrogen bonds, while faster components are associated with methyl group motions and structural relaxation. Ongoing molecular dynamics simulations are used to calculate dynamic structure factors and support the interpretation of neutron and dielectric spectroscopy data, with the goal of disentangling the individual relaxation processes. Together, these experimental and computational efforts provide detailed insight into the pressure-, concentration-, and temperature-dependent hydrogen-bond dynamics of mono-hydroxy alcohols.

**b0032**

**In-situ High Temperature Raman Spectroscopic Study of Glycine:Urea 1:1 Co-crystal Revealing Fluorescence Activation**

Harsha Kumawat,[1,4] Himal Bhatt,[1,4,a)] S.R. Vishwakarma,[1]Shovit Bhattacharya,[2,4] L. Panicker,[3] T. Sakuntala[1,4]
[1]*High Pressure & Synchrotron Radiation Physics Division,*
[2]*Technical Physics Division,*
[3]*Protein Crystallography Section, Bhabha Atomic Research Centre, Trombay, Mumbai, India 400085*
[4]*Homi Bhabha National Institute, Anushaktinagar, Mumbai, India 400094*
[a)]*Email:hbhatt@barc.gov.in*

In this work, we report the first Raman spectroscopic study of a 1:1 co-crystal of glycine and urea, with complete mode assignment. Further, in-situ high temperature Raman spectroscopy was carried out to study changes in molecular structure upon heating. The co-crystal was found to remain structurally stable up to ~140 °C, as evidenced by minimal Raman spectral changes. Beyond this temperature, a distinct fluorescence emerges, marking a thermally activated emissive state before it finally degrades at sufficiently high temperatures. This thermally activated fluorescence, highlights the potential of the glycine–urea adduct for applications in thermal sensing, photonics, smart warning labels and stimuli-responsive materials.

**b0033**

**Intelligent Multifunctional Hydrogel for Soft Robotic Applications**

KhashtiDatt Pandey[1a], Ankush Kumar[1], Ajay D. Thakur[1]
[1]*Department of Physics, Indian Institute of Technology Patna, Bihta 801106, India*
[a)]*Email:khashti_2121ph05@iitp.ac.in*

Intelligent multifunctional hydrogels are versatile polymeric materials. These are soft and compact materials that have various capabilities with excellent stimulus response. These have potential for applications in domains such as energy harvesting,

biomedical, soft sensors, micro biomechanics, and soft robots for medical care, etc. In this work, we synthesize a polyvinyl Alcohol (PVA), poly(vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP), and graphene oxide (GO) based multifunctional piezoelectric hydrogel, using organic solvents. This study explores the piezoelectricity and piezo-resistivity of the hydrogel. The piezoelectric response of the hydrogel was observed for constant force tapping, and piezo-resistivity has been demonstrated by strain-sensing capability.

**b0034**

**Polymer−MXene−Viologen-Based Suprahybrid Electrochromic Device: Flexible Smart Window with Visible and Near-Infrared Switchability**

Saumya Srivastava[1,a], Bhumika Sahu[1], Divyansh Mishra[1], Love Bansal[1], Nikita Ahlawat[1], Deb Kumar Rath[1], Partha Sarathi Rout[1], Shivam Kumar[1], Sharmistha Singh[1], Pratishtha Pandey[2,b], and Rajesh Kumar[1,c]

*[1]Materials and Device Laboratory, Department of Physics, Indian Institute of Technology Indore, Simrol453552, India.*

*[2]Department of Science and Technology (DST), New Delhi 110016, India.*

*Email: a) phd2401151015@iiti.ac.in; b) pratishtha.tp@nic.in; c) rajeshkumar@iiti.ac.in*

This study demonstrates an advanced suprahybrid solid-state electrochromic device developed by combining materials from three different families: conducting polymer (P3HT), organic functional molecules (viologen), and 2D MXenes (V2C). The V2C MXene doping significantly enhances the performance of the polythiophene-viologen based device, achieving a color contrast of 38.4% with switching times less than 0.5 seconds. The device exhibits dual-range functionality, switching in both visible and near-infrared wavelengths, enabling heat reduction up to 12% in the ON state. High coloration efficiency exceeding 800 $cm^2/C$ and excellent cyclic stability for 2000 seconds demonstrate the device's practical viability. The flexible nature of the device was successfully demonstrated through prototype goggles capable of selective color switching for specialized applications including 3D vision systems. This work provides a promising approach for developing energy-efficient smart windows and flexible optoelectronic devices.

# c) Nano-materials

**c0001**

**Growth and Characterization of $(C_2H_5)_2ZnCl_4$ Hybrid Single Crystals for Nonlinear Optical Applications**

Preeti[a,] and Shobha Kulshrestha[b*]
[a]*Nims University Rajasthan Jaipur (India)*
[b]*Nims University Rajasthan Jaipur (India)*
**Corresponding author's email address: shobha.kulshrestha@nimsuniversity.org, preetigoyal94164@gmail.com*

The current study aims to explore the organic-inorganic hybrid material diethyl zinc chloride's ($(C_2H_5)_2ZnCl_4$) single crystal development and nonlinear optical (NLO) characteristics in order to comprehend its possible uses in photonic and optical devices. A slow evaporation approach was used to synthesize high-quality single crystals of $(C_2H_5)_2ZnCl_4$ with few defects to start the investigation. There is little impurity in the developed crystal and the crystallites have acceptable quality, thus we can say that the crystal structure is orthorhombic. FT-IR spectroscopy reveals that the linked chemical has many functional groups. In ultraviolet-visible spectroscopy, the optical band gap is determined. Considerable optical switching, frequency conversion and NLO responses are displayed by the material.

**c0002**

**Highly Responsive NiO/MCM-48 Humidity Sensor for Sleep Hypopnea- Apnea Detection**

Priya Malik[1,2 a)], Surender Duhan[1 b)], Ajay Kumar Sharma[2, c)], and Gyanendra Sheoran[2, d)]
[1]*Advanced Research in Optical and Microwave Applications (AROMA) Lab, Department of Applied Sciences, National Institute of Technology Delhi, Delhi, India*
[2]*Advanced Sensors Lab, Department of Physics, Deenbandhu Chhotu Ram University of Science and Technology, Murthal, (Sonipat)-131039, Haryana, India*
**[b), d)]Email: surender6561@gmail.com , gsheoran@nitdelhi.ac.in*

To identify Sleep Hypopnea-Apnea Syndrome (SHAS), a common sleep disorder characterized by breathing disruptions, a novel humidity sensor utilizing a NiO/MCM-48 nanocomposite has been developed. Scanning electron microscopy (SEM) verified that the hydrothermal synthesis of the NiO/MCM-48 composite produced distinct spherical nanostructures. The sensor utilizes the semiconducting qualities of NiO and the porous structure of MCM-48, both of which are critical for humidity detection. The sensor exhibits quick response and recovery times of 10.8 s and 9 s, respectively. In order to detect apnea episodes, it was also used in a real-time monitoring system to track changes in humidity associated with human breath.

**c0004**

**Exploring The Forster Resonance Energy Transfer between Ligand Protected Copper and Gold nanoclusters For Enhanced Photoluminescent Applications**

Shubhankar Narayan Bandekar and Sudhir Cherukulappurath
*School of Physical and Applied Sciences, Goa University, Taleigao Goa, 403203, India.*
**Email: sudhir.c@unigoa.ac.in*

Metal-enhanced fluorescence (MEF) and Förster resonance energy transfer (FRET) are synergistic photophysical phenomena that enable signal amplification and energy modulation in nanoscale systems. This study investigates the integration of MEF and FRET in hybrid copper–gold (Cu–Au) nanocluster assemblies, synthesized separately and combined post-synthesis. By leveraging the plasmonic properties of gold nanoclusters and the environmentally responsive fluorescence of copper nanoclusters, we demonstrate enhanced photoluminescence and tunable energy transfer behaviour. UV-Vis and PL spectroscopy reveal distinct spectral features. Silica shell engineering enables precise control over donor–acceptor spacing, optimizing both MEF and FRET efficiencies. These findings underscore the potential of Cu–Au nanoclusters as multifunctional platforms for biosensing, optoelectronic applications etc.

**c0006**

**Tailoring COK-19 Mesoporous Silica for Enhanced Cefepime Encapsulation and Sustained Release**

Anisha[1], Gyanendra Sheoran*[2], Surender Duhan*[1] and Priya Malik[1, 2]
[1] *Drug Delivery System Laboratory, Department of Physics, Deenbandhu Chhotu Ram University of Science and Technology, Murthal, Sonipat (131039), Haryana, India*
[2]*Advanced Research in Optical and Microwave Applications (AROMA) Lab, Department of Applied Sciences, National Institute of Technology Delhi, Delhi, India*
**Emails: gsheoran@nitdelhi.ac.in and drsurenderduhan.phy@dcrustm.org*

Mesoporous silica materials are leading the way in drug delivery systems based on nanotechnology. Mesoporous silica COK-19 has homogeneous pore size distribution, high surface area and good biocompatibility, which enabling the encapsulation and controlled release of drug molecules. This study looks into the development of a controlled drug delivery system by assimilating cefepime inside COK-19. Cefepime loaded COK-19 formulations were analyzed with UV-Vis spectroscopy, FTIR and BET. The release profile exhibits the sustained release of cefepime over a period of 72 hours. This scrutiny represents that COK-19 can be used as a vehicle for sustained and controlled drug delivery.

**c0007**

**Alteration Of Structural And Magnetic Properties Of $CoCr_xFe_{2-x}O_4$ Nanomaterials Synthesized By Citrate Autocombustion Method**

Anagha B. Patil[1] and Rabi N. Panda[1,*]

[1]*Department of Chemistry, Birla Institute of Technology and Science, Pilani, K K Birla Goa Campus, Zuarinagar, Sancoale, Goa 403726, India*

**Corresponding author: rnp@goa.bits-pilani.ac.in*

Synthesis of $CoCr_xFe_{2-x}O_4$ (x = 0.0, 0.1 and 0.3) nanomaterials were carried out using citrate autocombustion method. XRD analysis confirms the formation of pure cubic phase of the products annealed at 650 ºC. The average crystallite sizes (D) were 40 nm, 36 nm and 40 nm for x = 0.0, 0.1 and 0.3 in $CoCr_xFe_{2-x}O_4$, respectively. The lattice parameters show an overall decrease from 8.3551 Å to 8.3360 Å for x = 0.0 to 0.3, respectively. FTIR studies confirm the characteristic M–O bonding frequencies observed in range of 616 – 630 $cm^{-1}$ for $T_d$ site occupancy whereas 414 – 416 $cm^{-1}$ and 451 – 455 $cm^{-1}$ showing the $O_h$ site occupancy in all $CoCr_xFe_{2-x}O_4$ materials. The magnetic properties were studied using VSM measurements at 300 K. The significant linear decrease in the saturation magnetization ($M_s$) was from 74.3 emu/g to 60.7 emu/g for 'x' varying from 0.0 to 0.3 in $CoCr_xFe_{2-x}O_4$, respectively. The observed coercivity ($H_c$) values was 780 Oe to 453 Oe for x = 0.0 to 0.3, respectively. All the magnetic parameters studied in this work for $CoCr_xFe_{2-x}O_4$ nanomaterials could be correlated to the insertion of $Cr^{3+}$ ions in $CoFe_2O_4$, cation redistribution and size and surface effects.

**c0008**

**A Highly Selective Gas Sensor Based on $WO_3$/MCM-48 Nanocomposite**

Pankaj Kumar[1, a)], Gyanendra Sheoran[2, b)], Surender Duhan[1, c)], Priya Malik[1,2, d)]

[1] *Advanced Sensors Lab, Department of Physics, Deenbandhu Chhotu Ram University of Science and Technology, Murthal, Sonipat, Haryana-131039*

[2] *Advanced Research in Optical and Microwave Applications (AROMA) Lab, Department of Applied Sciences, National Institute of Technology Delhi, Delhi-110036*

[b), c)] *Corresponding author: gsheoran@nitdelhi.ac.in, drsurenderduhan.phy@dcrustm.org*

Gas sensing materials with high sensitivity and rapid response are essential for monitoring toxic gases in environmental and industrial applications. In this study, tungsten oxide-incorporated MCM-48 nanocomposite was successfully synthesized via an in-situ hydrothermal technique. Subsequently, a highly selective Carbon Monoxide (CO) based sensor was fabricated using the drop-casting approach. The structural characteristics of the synthesized material were analyzed using Wide-Angle X-ray Diffraction (WAXRD) within the 20°-80° 2θ range and Fourier Transform Infrared (FTIR) spectroscopy spanning 500-4000 $cm^{-1}$, confirming the formation of the intended nanocomposite. The fabricated sensor demonstrates a rapid response time of 21.3 seconds and a recovery time of 19.5 seconds at ambient temperature.

**c0009**

**Facile Synthesis of Microspherical $CuBi_2O_4$ a Promising Electrode for Next-Generation Supercapacitors**

Amisha[1], Aman Deep Acharya[1, a)], Yugesh Singh Thakur[1]

[1]*Department of Physics, Lovely Professional University, Phagwara, 144402 Punjab, India*

[a)] *Corresponding author: acharyaphysics2011@gmail.com*

In this study, Copper bismuth oxide ($CuBi_2O_4$) was synthesized via a facile co-precipitation method and investigated as a potential electrode material for supercapacitor application. XRD analysis confirmed the formation of $CuBi_2O_4$ in a pure phase, with no detection of extra peaks. The morphology of the prepared material exhibits a microsphere-like morphology offering a high surface area favorable for electrochemical properties. In contrast, electrochemical properties were studied in 6 M KOH, exhibiting specific capacitance of 614.33 F/g and 572.82 F/g at 10 mV/s and 1 A/g, respectively, making it promising electrode material for supercapacitors.

**c0011**

**Synthesis of Hydrothermal routed BiOCl hierarchical nanostructures and their exceptional photocatalytic properties**

Gokulakrishna R[1], S. E. Minhaaj[1], N. Abdul Kalam[1], L. Allwin Joseph[1, a)]

[1]*Department of physics, The New College, Chennai 600 014, India.*

[a)]*Corresponding Author: allwin@thenewcollege.edu.in*

Bismuth oxychloride (BiOCl) nanomaterials were synthesized via the hydrothermal method and systematically characterized to assess their photocatalytic properties. Structural analysis using XRD confirmed the formation of phase-pure, tetragonal BiOCl with high crystallinity. UV-vis DRS spectra reveal strong optical absorption in the UV region, indicating a moderate bandgap suitable for photocatalytic activity. FTIR and FT-Raman identified characteristic vibrational modes, confirming the chemical structure and purity of the BiOCl samples. The Photocatalytic performances were evaluated by the photocatalytic degradation of methyl orange under Xenon lamp irradiation. BiOCl showed good photocatalytic activities with almost all of the Methyl orange degraded in 60 min. This work provides a facile and accessible pathway to design effective photocatalysts for photocatalytic degradation.

**c0012**

**Investigating the Role of Enhanced Surface Area of Dry Electrodes on the ECG Signal Quality**

C. M. Vidhya[1, a)], Lakshay Bhardwaj[1], Shivam Singh[1], J. P. Singh[1]

*Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, 110016, India.*
**Email:vidhyacm21@gmail.com*
Accurate and noise-free Electrocardiogram (ECG) monitoring is essential for clinical diagnosis and in wearable ECG devices. There are several factors that affect the ECG signal quality, with the low skin-electrode interface impedance being a key parameter. This study investigates the effect of enhanced electrode surface area on the skin-electrode impedance and ECG signal quality. A comparison between silver thin-film electrodes and nanostructured silver nanorod-based electrodes was performed, which were fabricated by the glancing angle deposition technique (GLAD). Human trials were conducted using both electrode types. Results show that electrodes with a larger effective surface area exhibit significantly lower skin-electrode impedance compared to the flat thin-film electrodes. ECG signal quality assessed using signal-to-noise ratio was higher for silver nanorod electrodes (12 dB) than the silver thin film electrodes (8.8 dB). These findings highlight the role of surface engineering to improve the performance of dry electrodes, providing better quality ECG signals and offering valuable insights for the development of high-fidelity wearable biosensors.

**c0014**

**Ferrites Based Magnetic Nanostructured Materials for Waste-water Treatment**

Naresh Prajapati and Himanshu Pandey *
*Condensed Matter & Low-Dimensional Systems Laboratory, Department of Physics,*
*Sardar Vallabhbhai National Institute of Technology, Surat 395007, India.*
**Email:hp@phy.svnit.ac.in*
Advanced oxidation processes such as photocatalysis are widely explored to tackle such problems. In photocatalysis, highly oxidative species such as hydroxyl radicals (*OH) are produced using semiconducting photocatalysts and light. A photocatalyst decomposes the toxic organic compounds in the presence of light. The semiconducting ferrite-based nanostructures are an essential candidate as a photocatalyst due to their narrow optical bandgap. These nanostructures, such as nanoparticles and nanofibers, possess many advantages, such as accessible pore structure and ease of surface modification. In this work, we report on the structure, morphology, and optical characterization of cobalt ferrite nanoparticles and nanofibers. The photocatalytic activity of these nanostructure materials was investigated using methyl orange and methylene blue aqueous solutions as a model dye and a low-power white LED as a light source, resulting in a decomposition of around 95 % of the dye after 150 minutes of irradiation. The *OH radicals were identified as the main reactive species. Also, the recyclability tests showed that the photocatalyst can be used multiple times without compromising its efficiency.

**c0015**

**Structural, Optical, Morphological, Photo-catalytic and Antioxidant activities Of Green Synthesized Ag doped ZnO Nanoparticles By Using Orange Peel**

Amarjot Kaur[1a], Atul Khanna[2], Harpreet Kaur[1] and Randhir Singh[1]
[1]*Department of Applied Sciences, Guru Nanak Dev Engineering College, Ludhiana, 141004, Punjab, India*
[2]*Department of Physics, Guru Nanak Dev University, Amritsar, 14305, Punjab, India*
*Email: *as_amarjot@gndec.ac.in ; amarjotphy4@gmail.com*
This study explores the green synthesis of Ag-doped ZnO nanoparticles using orange peel extract as a natural reducing and stabilizing agent. Structural and morphological characterization confirmed hexagonal wurtzite structure and uniform Ag distribution. The optical band gap decreased from 3.40 eV to 2.99 eV with Ag doping. Photocatalytic activity reached 90.99% dye degradation, and antioxidant activity also improved significantly. These results highlight the enhanced multifunctional properties of Ag-doped ZnO NPs for environmental and biomedical use.

**c0016**

**Sol-gel Synthesis and Crystallographic Study of ZnO/f-MWCNTs Nanocomposites**

Babli Kumari[1], Atul Yadav[2], Punit K. Dhawan[2], Ratnesh K. Pandey[3], Shikha Awasthi[1]*
[1]*Department of Physics, M. M. Mahila College, Veer Kunwar Singh University, Ara, Bihar, India- 802301*
[2]*Department of Physics, Prof. Rajendra Singh (Rajju Bhaiya) Institute of Physical Sciences for Study &Research, V.B.S. Purvanchal University, Jaunpur, UP, India- 222003*
[3]*Department of Physics, University of Petroleum and Energy Studies (UPES), Dehradun, Uttarakhand, India-248007*
**Email: awasthi.shi@gmail.com*
Zinc oxide nanoparticles (ZnO NPs) and functionalized multi-walled carbon nanotubes (ZnO/*f*-MWCNTs) nanocomposites were successfully synthesized using the Sol-gel method. The incorporation of ZnO onto the surface of *f*-MWCNTs led to a composite material exhibiting significantly enhanced electrical, optical, catalytic, and sensing properties as compared to bare ZnO nanoparticles and MWCNTs. The crystallographic properties of ZnO nanoparticles, *f*-MWCNTs, and ZnO/*f*-MWCNTs nanocomposites were investigated using X-ray diffraction (XRD) techniques. The XRD patterns confirmed the presence of a hexagonal wurtzite crystal structure. ZnO/*f*-MWCNTs nanocomposites exhibit an average crystallite size of 36 nm, calculated using the Debye-Scherrer equation, confirming their crystalline nature. This study has potential future applications in the fields of science & technology and industry.

**c0017**

**Scanning Probe-Based Insights and Laser-Driven Modulation Studies Of Graphene Oxide**

Namita Rane[1, a)] , Sugam Kumar[2], V.K. Aswal[2] and Sudhir Cherukulappurath[1,b]
[1]*School of Physical and Applied Sciences, Goa University.*
[2]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai, Maharashtra*
** Corresponding author: sudhir.c@unigoa.ac.in*

Graphene oxide (GO), a chemically functionalized graphene derivative, exhibits tunable electrical and optical properties due to its partially oxidized $sp^2$ carbon lattice. We investigated the nanoscale electrical and electromechanical properties of GO using C-AFM (conductive atomic force microscopy), PFM (piezoelectric force microscopy), and KPFM (Kelvin probe force microscopy), revealing enhanced conduction (~265 nA) in thinner flakes, a piezoelectric coefficient ($d_{33}$~0.59 pm/V), and a work function of ~4.80 eV. In addition, we investigated laser irradiation at 785 nm, which induced spatially selective partial reduction, improving conductivity and restoring $sp^2$ domains as confirmed by XPS. In contrast, thermal annealing led to complete deoxygenation but lacked spatial control, highlighting the tunability of laser processing for functional GO engineering.

**c0018**

**Passivation Effects of Potassium Bromide Doping in Cesium Bismuth Bromide Nanosheets**

Fency Sunny[1], Nandakumar Kalarikkal [1,2,3,a)], Subila K. B.[4,b)]
[1]*International and Inter University Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University, Kottayam-686560, Kerala*
[2]*School of Pure and Applied Physics, Mahatma Gandhi University, Kottayam-686560, Kerala*
[3]*International Centre for Ultrafast Studies, Mahatma Gandhi University, Kottayam-686560, Kerala*
[4]*School of Chemical Sciences, Mahatma Gandhi University, Kottayam-686560, Kerala*
[a)] *Corresponding author: nkkalarikkal@mgu.ac.in*
[b)] *Corresponding author: subila@mgu.ac.in*

Lead-free halide perovskites have garnered increased scientific rigor owing to the feasible non-toxic alternate they provide for lead based halide perovskite. Out of the various greener alternate, Bismuth based vacancy ordered perovskites have occupied a prominent position in optoelectronic applications. However, the efficiency of bismuth-based perovskite devices require improvement owing to the concentration of defects in this indirect bandgap material. Potassium doping has been proven to have defect passivation effect on lead-based halide perovskite. This study focuses on implementing this supposition in cesium bismuth bromide nanosheets and evaluate the effect of potassium incorporation in cesium bismuth bromide nanosheets. The structural, morphological and optical characteristics of the pristine and doped samples are assessed pointing to the improvement in optical properties as the doping concentration is increased. The study effectively shows the use of monovalent dopants for property enhancement and defect passivation.

**c0019**

**Development of Flexible SIS Nanocomposites with Enhanced Thermal Resistance via Hybrid Oxide Nanofillers**

Sangeetha Vijayagopal[1], Vengatesh Panneerselvam[2], Sanjeevi Prasath Sridhar[1]*
[1]*Soft Matter Laboratory, Centre for Nanoscience and Nanotechnology, Sathyabama Institute of Science and Technology, Chennai 600 119, Tamil Nadu, India.*
[2]*Centre of Excellence for Energy Research, Sathyabama Institute of Science and Technology, Chennai 600 119, Tamil Nadu, India*
**Email ID: sanjeeviprasath.irc@sathyabama.ac.in*

In this study, GO, $Fe_3O_4$, and NiO nanoparticles were synthesized and fabricated into $Fe_3O_4$-NiO and GO-$Fe_3O_4$-NiO nanocomposites via ball milling. The nanocomposites were incorporated into a styrene-isoprene-styrene (SIS) triblock copolymer to form flexible composite sheets. Thermal stability was assessed by thermogravimetric analysis (TGA), while XRD and Raman spectroscopy confirmed structure and phases. BET analysis measured surface area and porosity, and FESEM examined the surface morphology. The study aims to understand the impact of inorganic nanofillers on enhancing thermal resistance in SIS based flexible materials.

**c0020**

**Near-Infrared Activated $LaF_3$ Upconversion Nanoparticles for Deep-Tissue Imaging**

Pratik Deshmukh[1,2,a)], Bhumika Sharma[1], S. Satapathy[1,2], S. K. Majumder[1,2]
[1] *Functional Bio-Materials Lab., Laser Biomedical Application Division, Raja Ramanna Centre for Advanced Technology, Indore, India-452013*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai,Maharashtra, India - 400 094,.*
[a)]*Email: ppdeshmukh@rrcat.gov.in*

Upconversion nanoparticles (UCNPs) have emerged as promising probes for in vivo fluorescence imaging due to their unique ability to absorb near-infrared (NIR) light within the 900–1200 nm biological window. This property significantly reduces tissue autofluorescence and enhances imaging depth. In this research, lanthanide-doped $LaF_3$ UCNPs were synthesized and surface-modified with human serum albumin (HSA) to improve their water dispersibility and biocompatibility for biomedical use. Dynamic light scattering (DLS) measurements indicated particle sizes ranging from 20 to 30 nm. Under 980 nm laser excitation, these nanoparticles exhibited strong emissions in the visible range, particularly around 542 nm (green) and 656 nm (red), attributable to

energy transfer processes involving $Yb^{3+}$ ions. Stability in biological media was confirmed through zeta potential analysis in DMEM, and in vitro assays with HeLa cells demonstrated minimal cytotoxicity. These results support the application of HSA-coated $LaF_3:Ln^{3+}$ UCNPs as effective and biocompatible agents for deep-tissue NIR bioimaging.

**c0021**

**X-Ray K-Absorption Spectral Studies of Transition Metal Complexes At Nickel K-Edge**

Humera Khan[1], Pramod Kumar Malviya[2]
*[1]School of Studies in Physics, Vikram University Ujjain (M.P) India*
*[2] Govt Madhav and Science College Ujjain (M.P) India*
*E-Mail:- humerakhan23nov@gmail.com*

In the present investigation, XANES and EXAFS data of transition metal complexes, i.e., complex **I** – $[Ni_{0.8}Cu_{0.2}Fe_2O_4]$, complex **II** - $[Ni_{0.6}Cu_{0.}4Fe2O4]$ and complex **III -** $[Ni_{0.4}Cu_{0.6}Fe_2O_4]$ have been analyzed. The K-edge has been found to split into two components, i.e., $K_1$ and $K_2$ in all of these complexes. From these, the shift of the $K_1$-edge (chemical shift), shift of the principal absorption maximum, ENC and edge-width has been obtained. On the basis of values of the chemical shifts, all studied complexes have oxidation state +2. The chemical shift has been used to determine the effective nuclear charge on the absorbing atom. From the positions of the EXAFS maxima and minima, the bond lengths in the complexes have been determined by three different methods viz. Levy's, Lytle's and Lytle, Sayers and Stern's (L.S.S.) methods. From the Fourier transforms of the EXAFS spectra the bond lengths (uncorrected for phase shift) have been determined. It has been observed that the value of the phase uncorrected bond length, i.e., $(R_1-\alpha_1)$ as determined from L.S.S. method and that determined from the Fourier transformation method are in good agreement with each other $R_1$. The XANES and EXAFS data have been analyzed using Origin 2019 and Athena software.

**c0022**

**Stability Evaluation of Nanostructured AAO-Au Substrates for SERS Applications**

Najneh H. Dehkordi and Rajeshkumar S. Hyam
*School of Physical and Applied Sciences, Goa University, Taleigao, Goa, India. 403206*
**rajesh.hyam@unigoa.ac.in*

For precise and accurate sensing applications, substrates must maintain stability over time and across different conditions. This makes the stability of Surface-Enhanced Raman Scattering (SERS) substrates especially important, as it directly affects their performance and durability in real-world environments. This study evaluated the Raman signals of gold nanoparticles (AuNPs) coated on porous anodic aluminum oxide (PAAO) thin films with three different pore lengths on day 1 and day 30 to assess their stability. Formation and uniformity of the AAO thin films were confirmed by scanning electron microscopy (SEM). The sample S1, which has a shorter pore length than samples S2 and S3, demonstrated exceptional signal stability with a slight increase (~6.3%) in SERS intensity after 30 days. This suggests potential self-enhancement effects, which may be attributed to a gradual increase in analyte attachment, better exposure of plasmonic hot spots, or slight surface changes that make the substrate more favorable for molecular interaction.

**c0024**

**Assembling of Atomic Gold Clusters to Photodetector Devices**

Satchidananda Rath[(a)] and Pragyan Paramita Dash
*School of Basic Sciences, Indian Institute of Technology Bhubaneswar, Argul, Jatni-752050, Odisha, India*
*[(a)]Corresponding author: srath@iitbbs.ac.in*

Atomic metal clusters are compelling research subjects due to their tunable properties arising from atomicity-dependent electronic structures. Gold clusters and their superstructures with different atomicity have been pursued for decades due to their wide applications in optics. This work demonstrates the ligand-mediated assembling of eight atoms of gold clusters ($Au_8$) into a local periodic nanostructure. Structural characterization through transmission electron microscopy, X-ray diffraction, and small-angle X-ray scattering confirms a local periodicity of 1.47 nm in a hexagonal+1 arrangement of $Au_8$ clusters. The observation of two opposite natures of the excitonic states in the circular dichroism spectra corroborates the coupling of excitons with distinct chirality. The magnetic behavior, supported by both theoretical and experimental analysis, exhibits super paramagnetic ordering driven by spin-orbit interaction. Additionally, the discretization of the electronic states and spin-orbit coupling resulted in a promising HOMO-LUMO gap, functioning as a semiconductor. The Schottky junction-based device demonstrates a distinct photoresponse in the ultraviolet region, marking a significant advancement in the development of next-generation UV-sensitive photodetectors.

**c0025**

**A Machine Learning-assisted Model for Predicting the Crystallinity of Cellulose Nanocrystals**

Deepa Sreedev[1,a)], Nandakumar Kalarikkal[1,3,4,b)], Subila Kurukkal Balakrishnan[1,2]
*[1] International and Inter-University Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University, Kottayam-686560, Kerala, India*
*[2] School of Chemical Sciences, Mahatma Gandhi University, Kottayam-686560, Kerala*
*[3]School of Pure and Applied Physics, Mahatma Gandhi University, Kottayam 686560, Kerala*
*[4]International Centre for Ultrafast Studies, Mahatma Gandhi University, Kottayam-686 560, Kerala, India*
*[a)]deepasdev1989@gmail.com [b)] nkkalarikkal@mgu.ac.in*

Cellulose nanocrystals (CNCs) exhibit varying degrees of crystallinity depending on their source and processing conditions, which significantly influence their properties. Traditional methods such as XRD, NMR, and FTIR often yield inconsistent measurements of CNC crystallinity, making characterization challenging. To address this, a machine learning model was developed using literature data, incorporating various cellulose sources and reaction conditions as inputs. Among several regression models tested, including Support Vector Regressor (SVR) and Random Forest, the K-Nearest Neighbours (KNN) model achieved the best performance, with an $R^2$ of 0.82 and RMSE of 1.59. This demonstrates that machine learning can reliably estimate CNC crystallinity based on processing parameters.

**c0026**

**Characterization and Biocompatibility Assessment of Collagen-Hydroxyapatite Scaffolds for Tissue Engineering Applications**

Kanika Chandel[1], Kulwinder Kaur[2,3], Gurdev Preet Singh[1], K.J. Singh[1,a)]
[1] *Department of Physics, Guru Nanak Dev University, Amritsar, 143005, India*
[2] *School of Pharmacy and Biomolecular Sciences, Royal College of Surgeons (RCSI), Dublin D02 YN77, Ireland*
[3] *Tissue Engineering Research Group, Department of Anatomy and Regenerative Medicine RCSI Dublin D02 YN77, Ireland*
[a)] *Corresponding author: kanwarjitsingh.phy@gndu.ac.in*

Collagen-hydroxyapatite (HA) composite scaffolds were fabricated using the freeze-drying method for potential application in bone tissue regeneration. Structural and morphological characterization was carried out using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and filed emission scanning electron microscopy (FESEM) techniques. XRD analysis confirmed the formation of hydroxyapatite with well-defined peaks and FTIR spectra showed characteristic functional groups of both collagen and HA, indicating successful composite formation. FESEM images revealed a highly porous and interconnected structure, which is beneficial for cell infiltration and nutrient diffusion. The biocompatibility of the scaffolds was evaluated through an *in vitro* MTT assay using mesenchymal stem cells (MSCs), which showed good cell viability and proliferation over a 7-day culture period. These results suggest that the freeze-dried collagen-HA scaffold is a promising candidate for bone tissue engineering applications.

**c0027**

**Influence of Low-Concentration Thallium Doping on the Structural, Optical, and Transport Properties of $Bi_2Se_3$ Nanoparticles**

Hitesh Chaudhary[1], Archana Lakhani[2], Ashwini Mahadik[3], Dhruti Bhagora[1] and P. H. Soni[1,*]
[1]*Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara 390002, India.*
[2]*UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore 452001, India.*
[3]*Parul Institute of Engineering & Technology, Parul University, Limbda, Vadodara- 391760, India.*
**Email: ph.soni-phy@msubaroda.ac.in*

$Bi_{1.98}Tl_{0.02}Se_3$ nanoparticles were synthesized via the hydrothermal method and characterized to investigate the effects of low-level thallium doping on $Bi_2Se_3$. XRD analysis confirmed a hexagonal crystal structure, FTIR spectra indicated Bi(Tl)–Se vibrational modes, and the optical band gap was found to be 1.187 eV from DRS analysis. Electrical transport measurements conducted in the range of room temperature to 430 K showed a negative Seebeck coefficient, increasing in magnitude from –60 μV/K at room temperature to –78 μV/K at 430 K. The power factor also improved with temperature, reaching $0.39\times10^{-3}$ $Wm^{-1}K^{-2}$ at 430 K, indicating promising thermoelectric potential. These findings demonstrate that even low-concentration thallium doping can effectively optimize the thermoelectric properties of $Bi_2Se_3$ for energy conversion applications.

**c0028**

**Green Route To Blue Emission: Rare Earth Doped Amorphous Silica From Agriculture Waste**

Anjali Bala[1], and Arvind k Gathania Gathania[1, a)]
[1]*Department of Physics and Photonics Science, National Institute of Technology Hamirpur, 177005 (H.P.) India*
**Email: akgathania@nith.ac.in*

Solid-state reaction method was used to prepare the Tb3+ doped amorphous silica (SiO2: x Tb3+) samples with various concentrations, x = 0, 1, 2, 3, 4, 5 mol %. The method of extraction of SiO2 from groundnut shells (GS) is easy, involving only two steps, and eco-friendly. To confirm the amorphous phase of prepared SiO2, the X-ray diffraction (XRD) analysis was used. The FTIR study was carried out for the analysis of chemical bonds present in the prepared samples. The optical properties were investigated with photoluminescence studies. The maximum Pl intensity on excitation of 243 nm was observed for SiO2: 2 mol% Tb3+ with chromaticity coordinates (0.2159, 0.1780) and color purity (CP) 56.2% giving blue light emission. The blue light emitting phosphor materials have uses in lighting and photonics devices.

**c0029**

**Mass Spectrometric Characterization, Density Functional Theory and Photoionization Investigations of Copper Doped Subnanometer Sized Yttrium Monoxide Clusters**

Varun Vinayak Deshpande,[1,2 a)] Vaibhav Chauhan,[1] Chaithanya P. Bhat,[3]Debashis Bandyopadhyay,[3] and Soumen Bhattacharyya.[1,2]
[1]*Bhabha Atomic Research Centre, Trombay, Mumbai, India.*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai, India*

[3]*Birla Institute of Technology, Pilani, Rajsthan, India*
[a)] *Corresponding author: varund@barc.gov.in*
Subnanometer sized copper doped yttrium monoxide clusters were produced in a recently built metal cluster beam setup by gas phase chemical reaction of laser vaporized Y and Cu metal plasma with oxygen followed by supersonic cooling in a helium gas expansion. Laser photoionization and Reflectron Time of Flight Mass Spectrometry (Re-TOFMS) were used to investigate the mass spectrometric stability and to calculate Threshold Ionization Energy (TIE) of oxygen deficient neutral $Y_mOCu$ (m = 2— 4) clusters. Adiabatic Ionization Energy (AIE) for $Y_mCuO$ (m=2— 4) clusters with their lowest energy structures was calculated by employing Density Functional Theory (DFT) methods. Reasonable agreement between the theoretically calculated AIE and TIE is obtained for the $Y_mCuO$ (m=2— 4) clusters. The comparison of TIE of $Y_{m+1}O$ and $Y_mOCu$ cluster reveals the effect of the copper atom doping on the electronic stability of $Y_mO$ clusters.

**c0030**

**Structural, Optical And Photocatalytic Studies Of Bismuth Oxybromide Nanoparticles**

S.E. Minhaaj[1], Gokulakrishna R[1], L. Allwin Joseph,[1*]Abdul Kalam N[1]
[1]*Department of physics, The New College, Chennai 600 014, India.*
[a)] *Corresponding Author: minhaaj0211@gmail.com*
[b)] *Corresponding Author: gokulramesh4101@gmail.com*
[c)] *Corresponding Author: allwin@thenewcollege.edu.in*
The current work is focused on investigating the result of Bismuth Oxybromide nanoparticles synthesized by hydrothermal method. The detailed structural, compositional and optical characterizations of the synthesized BiOBr nanoparticles were characterized by X-ray diffraction (XRD), UV-Vis spectroscopy, Plotoluminescence (PL), Fourier Transform Infrared Spectroscopy (FTIR) and FT-Raman, and Photocatalytic studies. X-ray diffraction analysis confirmed the phase purity and high crystalline nature of the synthesized sample. The optical property of the synthesized material was analyzed using UV spectral analysis and the band gap for BiOBr was found to be 2.98 eV respectively. FTIR and FT Raman vibrationnal spectroscopic techniques used for chemical and structural analysis. PL to analyze the optical and electronic properties of BiOBr. Under Xenon lamp irradiation, the photocatalytic degradation of rhodamine B was used to assess the photocatalytic capabilities. In 75 minutes, nearly all of the rhodamine B was fully degeraded by BiOBr, demonstrating strong photocatalytic activity.

**c0031**

**Spectral Properties of Rare-Earth-Doped Fullerenes: Insights from Time-Dependent Density Functional Theory**

Munendra Jain, Sheetal Sisodiya
*School of Technology Management & Engineering, SVKM`s NMIMS, Indore-453112*
**Email:mjain03@yahoo.com*
The fullerene molecule has very interesting and useful electronic and conductive characteristics, which are depending upon the genre of doped substance. Therefore, it is becoming the most research preferred area of Nano technology and allied fields. we have used a rare earth-doped (Europium) fullerenes C60 molecules to report its electronic and conductive properties with different parameters. Lanthanides have always given new dimensions and directions to research due to their properties. In present study, we have used time dependent density functional theory-based approach for better understanding and new possibilities of Rare Earth-Doped Fullerenes.

**c0032**

**Synthesis of Binder-Free $Ni_3S_2$ for Supercapacitor Applications**

Kritika Yadav[1], Aman Deep Acharya [1, a)], Yugesh Singh Thakur[1], Amisha[1]
[1]*Department of Physics, Lovely Professional University, Phagwara, 144411 Punjab, India*
[a)] *Corresponding author: acharyaphysics2011@gmail.com*
In this study, one-pot hydrothermally synthesized nanostructured granular-like $Ni_3S_2$ was used as electrode material for advanced supercapacitors. Structural and morphological characterization of $Ni_3S_2$ electrode was determined using X-ray diffraction (XRD), and field emission scanning electron microscopy (FESEM). Surface morphology shows granular nanostructure on the surface of Ni substrate. XRD analysis confirms the formation of a high-purity phase and crystallinity of $Ni_3S_2$. The electrochemical behaviour of synthesized $Ni_3S_2$ electrode was analysed by cyclic voltammetry (CV), and galvanostatic charge-discharge (GCD). Analysis showed at 1 $Ag^{-1}$ current density 6 M KOH exhibits enhanced capacitance of 1542.5 $Fg^{-1}$. The $Ni_3S_2$ nanostructured electrode exhibits excellent electrochemical properties due to its sufficient electroactive sites for redox action and a promising electrode material for supercapacitor applications.

**c0033**

**Visible-Blind UV-C Photodetection Using NiO-ZnO Nanorods on a Flexible Substrate**

Vaishnavi K Mohan[1] and Teny Theresa John[1, *]
[1] *Department of Physics, Birla Institute of Technology and Science, Pilani, K K Birla Goa Campus, Zuarinagar, Sancoale, Goa 403726, India*
[*] *teny@goa.bits-pilani.ac.in*

A flexible, visible-blind ultraviolet (UV) photodetector was fabricated using NiO–ZnO (NZ) nanocomposites, consisting of one-dimensional ZnO nanorods with a hexagonal wurtzite structure decorated with cubic NiO quantum dots (QDs). The device shows a significant photocurrent response under UV-C illumination, even at low light intensity, while remaining insensitive to visible light.

**c0034**

**Optimization of Bath Temperature for Electrodeposited NiFeWMoMn High-Entropy Alloy Thin Films**

Divya V [1], Kannan R [2], Sengodan R [3*]

*[1,3*]Department of Physics, School of Foundational Sciences, Kumaraguru College of Technology, Coimbatore – 641 049, Tamil Nadu, India*

*[2] Department of Physics, Sakthi Polytechnic College, Nachimuthupuram, Sakthinagar, Anthiyur (T.K), Erode (DT) – 638 315. sengodan.r.sci@kct.ac.in*

In this study, NiFeWMoMn high-entropy alloy thin films were successfully synthesized using the electrodeposition method by varying the bath temperature. The structural, surface, corrosion, magnetic, and compositional properties were thoroughly analyzed using XRD, FESEM, EDS, electrochemical tests, and VSM. XRD analysis confirmed the formation of a solid solution with a refined crystalline structure, showing the smallest crystallite size and lower dislocation density at 75 °C. FESEM images revealed uniform and dense surface morphology at this temperature, while EDS confirmed the presence of all intended elements with a more balanced atomic distribution. Electrochemical corrosion studies showed that the sample coated at 75 °C exhibited the lowest corrosion rate and the highest polarization resistance, indicating superior corrosion resistance. Magnetic measurements showed that coercivity increased with temperature.75 °C was identified as the most favorable temperature for achieving uniform coating, better corrosion resistance, controlled magnetic behavior, and enhanced structural properties.

**c0035**

**Synthesis of Highly Pure Red Light- Emitting $CuSnI_3$ Quantum Dots by Modified Hot Injection Method**

Aryamol Stepehen[1,2], A. Biju[2] and P. M Sarun*[1]

*[1]Functional Ceramics Laboratory, Department of Physics, Indian Institute of Technology (Indian School of Mines), Dhanbad 826004, India.*

*[2]Materials and Condensed Matter Physics Laboratory, Department of Physics, MES Ponnani College, Calicut University, Ponnani, Malappuram, Kerala,679586, India.*

**sarun@iitism.ac.in*

We report the synthesis and optical characterization of novel $CuSnI_3$ quantum dots using a modified hot injection method without ligands. Structural analysis via XPS confirmed the presence of $Cu^+$, $Sn^{2+}$, and $I^-$ ions. HRTEM revealed nearly spherical particles with an average size of 3.1 ± 0.57 nm. Photoluminescence (PL) studies showed broad, multi-peaked emission in the visible range, with chromaticity coordinates (x = 0.6227, y = 0.3767) and 100% color purity, indicating strong red emission. This study introduces $CuSnI_3$ QDs as a promising, air-stable, lead-free material for optoelectronic applications.

**c0038**

**Structural, Photoluminescence and Photocatalytic Properties Of Semiconducting Graphitic Carbon Nitride (g-$C_3N$) Nanosheets**

Sangram Keshari Sahu[1], and Dojalisa Sahu[1*]

*[1]School of Applied Sciences, Centurion University of Technology and Management, Odisha, India*

**Email: dojalisa.sahu@cutm.ac.in*

This work presents a comprehensive analysis of the structural, photoluminescent, and photocatalytic properties of semiconducting graphitic carbon nitride (g-$C_3N_4$). X-ray diffraction (XRD) pattern exhibits a prominent (002) reflection at $2\theta \approx 27.4°$, corresponding to the interlayer stacking of conjugated aromatic systems, and a weaker (100) peak at $2\theta \approx 13.1°$, attributed to in-plane structural repeating units, confirming the graphitic layered structure. Field emission scanning electron microscopy (FESEM) reveals thin, crumpled nanosheets with homogeneous dispersion. Theoretical structural modelling using BioVia corroborates the observed crystallographic features with estimated optical bandgap (~3.02 eV) confirming semiconducting behaviour. Photoluminescence (PL) spectrum displays strong visible emission, indicative of effective charge recombination dynamics. Photocatalytic performance was evaluated by visible light induced degradation of Rhodamine B, monitored through absorption spectra. Kinetic analysis adheres to a pseudo-first-order model, reflecting efficient photocatalytic efficiency, supporting its applicability in environmental remediation.

**c0039**

**Understanding the Interaction Mechanism between Cyclo[12]carbon and Graphene Quantum Dots: A First-Principles Study**

L.K. Saini[1, a)], Ashvin Kanzariya[1]

*[1] Department of Physics, Sardar Vallabhbhai National Institute of Technology, Surat, India.*

*[a)] E-mail: lks@phy.svnit.ac.in*

In this investigation, we explore the interaction between Cyclo[12]carbon ($C_{12}$) and Coronene Graphene Quantum Dot ($C_{24}H_{12}$), two zero-dimensional carbon-based nanomaterials characterized by their unique structural and electronic properties. Our study consists of an in-depth analysis of their structural, electronic, and spectroscopic properties to determine the nature of their interaction. The separation between the $C_{12}$ nanocluster and Coronene GQD is found to be 3.37 Å, indicative of the close proximity. Furthermore, the negative interaction energy and the all-positive frequencies in the IR spectra provide compelling evidence for the stability of the newly formed complex structure. At last, RDG, NCI and QTAIM analysis indicate that the interaction between these two zero dimensional structures is van der Walls interaction.

**c0040**

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

S. Ilakiya[1] and P. Thangadurai[1,*]
[1]*Centre for Nanoscience and Technology, Pondicherry University, Kalapet, Puducherry- 605014, India*
[*]*Corresponding author: thangaduraip.nst@pondiuni.edu.in / thangadurai.p@gmail.com*

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

**c0041**

**Flow Synthesis of Nano-silica Impregnated Calcium Alginate Microsphere Using Droplet Microfluidics**

Nirvik Sen[1,3, a)], Ankit Ojha[1], Sugam Kumar[2,3] and Debasis Sen[2,3]
[1] *Chemical Engineering Division, BARC, Mumbai-400085*
[2] *Solid State Physics Division, BARC, Mumbai-400085,*
[3]*Homi Bhabha National Institute, Mumbai-400094*
[a)]Corresponding author: nirvik@barc.gov.in

A microbore tube-based droplet microfluidic platform is used to synthesize nearly uniform calcium alginate microspheres with impregnated nano-silica. 0.66 wt. % calcium alginate loaded with 0.66 wt. % of nano-silica aqueous dispersion was loaded onto a syringe pump. Precise droplets of this aqueous phase were generated in a 0.8 mm ETFE microfluidic T-junction using carrier phase as dodecane. A solution of $CaCl_2$ was used as the phase inversion/gelling agent. External gelation technique was adopted. Microsphere in the size range of 660 to 445 µm could be obtained as flow ratio of carrier to aqueous phase was varied from 20 to 30. Optical microscopy was used to quantify the morphology of the microspheres. Presence of nano silica in the microspheres were confirmed by Small-Angle Neutron Scattering technique (SANS). The structural correlation of the nano silica in the microspheres is quantified using SANS, which shows mass fractal kind of morphology of the embedded silica nanoparticles.

**c0042**

**Tailoring Structural, Thermal, Raman and Magnetic Properties of rare earth doped Nickel-Cobalt Ferrite Nanoparticles via a Low-Temperature Synthesis Route**

Hanamanta Badiger[1], [2*] and B.G. Hegde[2]
[1]*Department of Physics, Jain College of Engineering Belagavi-590014, Karnataka, India*
[2]*Department of Physics, Rani Channamma University Belagavi-591156, Karnataka, India*
**Email:hanamantabadiger93@gmail.com*

Rare-earth doping in spinel ferrites has gained attention as an effective strategy to tune their structural and other functional behavior for advanced magnetic and thermal applications. In this work, we report the successful synthesis of Yb doped nickel ferrite nanoparticles via a low-temperature sol-gel auto-combustion route for understanding their magnetic and thermal behavior. The diffraction pattern indicates a monophasic cubic spinel structure characterized by the Fd-3m space group. The Rietveld refinement analysis shows well-fitted Bragg reflections corresponding to a cubic spinel structure, indicating an increase in lattice constant and a decrease in crystallite size from 9 nm to 7 nm. The VSM-derived hysteresis loops at RT displayed a reduction in both magnetization and coercivity with increasing doping levels, suggesting a transition toward superparamagnetic behavior. TG–DSC analyses demonstrate a minimal weight loss of 2.96%, retaining 97.05% as residual mass upon rare-earth doping, suggesting improved thermal stability. The presence of five Raman-active modes corresponding to A1g, Eg, and F2g confirmed the structural fingerprint of the cubic spinel phase. These properties make the material suitable for thermal applications.

**c0043**

**Single-Step Synthesis of rGO and rGO/ZnO Composite Using Common Non-Toxic Precursors: Exploring a Wide Array of Applications**

Reshma S Philip, Meril Mathew*
*Department of Physics, St Joseph's College (Autonomous) Devagiri, Calicut-08, Kerala, India*
**meril.mathew@gmail.com*

Conventional chemical methods for synthesizing reduced graphene oxide (rGO) typically involve hazardous reagents, prolonged processing times, multiple steps, and generate toxic by-products. The synthesis of rGO/ZnO composites is even more complex, often requiring the separate synthesis of GO/rGO and its subsequent incorporation with zinc precursors or pre-formed ZnO via various techniques. In this context, we present a novel, single-step, and rapid method for synthesizing rGO/ZnO composites using inexpensive, non-toxic, and readily available materials. This scalable and energy-efficient process involves the pyrolysis of sucrose to form rGO, simultaneously with the decomposition of zinc acetate to produce the rGO/ZnO nanocomposite. The successful formation of rGO and the rGO/ZnO composite was confirmed using XRD, Raman spectroscopy, XPS, FE-SEM, HR-TEM, FT-IR, and UV–visible spectroscopy. The resulting composite exhibited promising performance in heavy metal adsorption, antibacterial activity, photocatalysis, and energy storage applications.

**c0045**

**Study of the Photo Response of Chemically Prepared Nanocomposite of Reduced Graphene Oxide/Zinc Oxide Nanoparticles at Room Temperature**

Ramesh Kumar[1,a], Amarjeet Kaur[2], Rajnish Kumar Yadav[1], Khushboo Mishra[1]
[1]*P.G Department of Physics, Veer Kunwar Singh University, Ara, Bihar - 802301, India*
[2]*Department of Physics and Astrophysics, University of Delhi, Delhi -110007, India*
[a)]*Corresponding author : rameshphysicsdu@gmail.com*

In this paper, we have synthesized a hybrid nanocomposite of reduced graphene oxide – Zinc oxide (rGO - ZnO). The Raman spectra of rGO – ZnO nanocomposite consists of characteristics peaks. Along with it, FTIR study confirms the characteristics peaks of rGO – ZnO nanocomposite. The SEM micrographs of the prepared samples show that ZnO nanoparticles stick on reduced graphene sheets which embedded in sample S4. The prepared samples tested for photo response measurement. It is observed that sample S4 exhibit a photo response of 7.25 % at 30 Mw/cm$^2$. The photo detection response seems to increase with concentration of ZnO. This is may be due to formation of P-N junction.

**c0046**

**Substrate Dependent Growth Study of $ZnIn_2S_4$ Nanostructures: Single Step Hydrothermal Approach**

Prashant K. Bankar
*Centre for Advanced Studies in Materials Science and Condensed Matter Physics, Department of Physics, Savitribai Phule Pune University, Pune – 411 007, India*
**Email:bankarprashant26@gmail.com*

The unique structural features and fascinating physicochemical properties of 2D nanostructured materials have shown great application in charge storage, optoelectronics and photoconduction device. Zinc Indium Sulfide (ZnIn2S4) is the only member of the ternary metal sulfides family with a layered structure. Amongst the methods used for synthesizing ZnIn2S4 structures, the hydrothermal technique offers a simple, cost-effective and environmentally friendly route for materials synthesis. To study the effect of substrate on the formation of hydrothermally grown ZnIn2S4 on several types of substrates were used. The structures of the ZnIn2S4 were systematically studied by scanning electron microscopy (SEM) and XRD. It was demonstrated that the type of substrates used had a great influence on the morphologies, density and alignment of the ZnIn2S4 formed. The ordered structure of nanometric dense ZnIn2S4 has been prepared on the conductive substrate for practical application in nano electronic devices.

**c0048**

**Flexibility Of ZIF-8 Under $CO_2$ Pressure Investigated by In Situ Positron Annihilation Lifetime Spectroscopy**

Jaideep Mor[1, 2] and Sandeep Kumar Sharma[1, 2, *]
[1]*Radiochemistry Division, Bhabha Atomic Research Centre, Mumbai 400 085*
[2]*Homi Bhabha Atomic Research Centre, Mumbai 400 094*
**Email:skumars@barc.gov.in*

We have investigated flexibility of Zeolitic Imidazolate Framework-8 (ZIF-8) under $CO_2$ pressure using in situ positron annihilation lifetime spectroscopy. It has been observed that open volume at pore sites is continuously reduced under $CO_2$ pressure for smaller size ZIF-8 crystals, whereas an enhancement in open volume at pore site is observed for larger size ZIF-8 crystals. The present study confirms that larger size ZIF-8 crystals behave as flexible whereas the smaller size ZIF-8 crystals behave as rigid framework under CO2 atmosphere.

**c0049**

**Characterization Of Ni and Cu Doped ZnO Nanoparticles**

Avneesh Kumar[1,]
[1]*Swami Vivekanand Govt. College Ghumarwin -174021, India*
**Email: 76avneesh@gmail.com*

In this article, exceptionally increase in production of nickel & copper doped zinc oxide nanostructures is reported. The ZnO nanostructures are synthesized with 10% of Ni & Cu doping adopting a Sol-gel method. Further the structural & crystallite size studies were performed by utilizing X-ray diffraction. The identification of wurtzite phase and determination of lattice parameters of Ni & Cu doped ZnO nanocrystallites is ascertained. X-ray diffraction (XRD) results indicate that the crystallite size is in 23-39

nm range, lattice parameters are a=0.32nm and c= 0.52nm respectively for wurtzite structure of ZnO. Also using UV-VIS spectroscopy of doped ZnO nanoparticles reveal absorbance and reflectance.

**c0050**

**Quantification of the pore structure in TEOS based Silica Aerogels doped with graphene oxide**

P. P. Govekar[1] , R. Raut Dessai[2, a)], D. Sen[3]
[1] *Department of Physics, PES's RSN College of Arts and Science Farmagudi Goa, 403401, India*
[2] *School of Physical and Applied Sciences, Goa University, Taleigao Plateau, Goa, 403206, India*
[3] *Solid State Physical Division, Bhabha Atomic Research Centre, Trombay Mumbai 400085, India*
**Email: reshma@unigoa.ac.in*

Silica aerogels doped with varying concentrations of graphene oxide (GO) were synthesized via a Two-Step Surface Modification method followed by Ambient Pressure Drying. The impact of GO incorporation on the pore morphology and structure of the aerogels was investigated. Pore volume, surface area, pore size, particle size, and radius of gyration were determined. Brunauer-Emmett-Teller (BET) analysis showed a maximum surface area of 541.7 $m^2/g$ for the sample containing 0.05 wt% GO. Small-Angle Neutron Scattering (SANS) revealed a highly interconnected porous network, with mass fractal dimensions ranging from 2.72 to 2.90. The results demonstrate that 0.05 wt% GO optimally enhances the structural features of silica aerogels, highlighting their potential for advanced energy storage applications.

**c0051**

**Resonance Photoemission in Mn:$CeO_2$ nanoparticles**

S. Tripathi[1,2,3,*,] Y. Kumar[1,2,] Mangla Nand[1,2,] Kiran Baraik[4] and Jaspreet Singh[2,5]
[1]*Beamline Development and Application Section, Bhabha Atomic Research Centre, Mumbai-400085, India*
[2]*BARC Beamline Section, Raja Ramanna Centre for Advanced Technology, Indore, India*
[3]*Homi Bhabha National Institute, BARC Training School Complex, Anushaktinagar, Mumbai-400094, India*
[4]*Accelerator Physics and Synchrotrons Utilization Division, Raja Ramanna Centre for Advanced Technology, Indore, India*
[5]*Technical Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, India*
**Email:shilpatripathi75@gmail.com*

The resonance photoemission observations on Mn doped $CeO_2$ nanoparticles prepared by chemical precipitation method are reported here. A comparative analysis of variable cerium valence states in the valence band of $CeO_2$ is an value addition in its electronic properties, as the relative contributions of $Ce^{3+}$ and $Ce^{4+}$ are found to shift upon Mn doping into the $CeO_2$ lattice. However, no change in the resonance photon energies (121 eV for Ce3+, while 124 eV for Ce4+) was observed upon doping. The effects of Mn incorporation are the reduction in Ce contribution and introduction of oxygen defects due to which the material becomes capable of storing and releasing oxygen atoms, which is useful in redox based applications such as gas sensing.

**c0052**

**Rare-Earth (Er, Tb) Doping-Induced Structural and Optical Modulation in Beta-Gallium Oxide Nanoparticles for Enhanced Blue Luminescence**

Abhishek Sharma [a)1] , Maneshwar Thakur[1] and Vir Singh Rangra [b)1]
[1] *Department of Physics, Himachal Pradesh University, Summer Hill, 171005, Shimla*
[a)] *Corresponding author; 00000abhisheksharma@gmail.com*
[b)] *veersinghrangra@gmail.com*

This study explores the structural and optical evolution of β-$Ga_2O_3$ nanoparticles doped with 1 wt.% $Er^{3+}$ and $Tb^{3+}$, synthesized via solid-state combustion method. X-ray diffraction (XRD) and Williamson-Hall (W-H) analysis confirm preservation of the monoclinic phase, along with a reduction in crystallite size and increased lattice strain upon doping. Raman spectroscopy reveals enhanced phonon damping and lattice disorder while retaining structural integrity. UV-Vis absorption spectra show an increase in band gap energy, which can be attributed to dopant-induced strain, lattice distortion, and the Burstein-Moss effect. Photoluminescence (PL) studies demonstrate notable enhancement in blue emission, with all samples exhibiting a dominant peak at 428 nm, attributed to intrinsic defect states such as oxygen vacancies ($V_O$), gallium vacancies ($V_{Ga}$), or vacancy complexes ($V_O$-$V_{Ga}$). The $Er^{3+}$ doped sample shows enhanced PL intensity compared to the undoped sample due to additional 4f transitions, while the $Tb^{3+}$ doped sample displays the most intense and well-resolved emission peaks among all three, including a distinct green emission at 544 nm corresponding to the $^5D_4 \rightarrow {}^7F_5$ transition. These findings underline the potential of rare-earth doped β-$Ga_2O_3$ for next-generation optoelectronic and photonic applications.

**c0053**

**In Silico Analysis of Cucurbit[6]uril–Cisplatin Inclusion Complex as a Drug Delivery Platform in Cancer Therapy**

Keka Talukdar
*Nadiha High School, Durgapur-713211, West Bengal, India*
**Email:keka.talukdar@yahoo.co.in*

Since it was approved as a cancer chemotherapeutic agent, Cisplatin is widely used in treating various cancers. But many unwanted side effects arising from poor solubility, off-target toxicity, and rapid deactivation in biological environments have restricted their use in reality. Inclusion complex of the drug with a macrocyclic host such as cucurbiturils enhances its efficacy by improving its

solubility and stability. In the current study, the formation of supramolecular cucurbit [6]uril (CB[6])–cisplatin inclusion complex and its activity as a nanocarrier system for cancer nanomedicine are investigated in detail. Molecular docking is performed to find the pockets of interaction, and the complex is formed with the most stable configuration. An explicit water model of the complex was generated, and molecular dynamics simulations were employed to evaluate the binding affinity, structural stability, and host–guest interactions within the complex. The findings support the use of CB[6] as a promising nanocarrier system for cisplatin delivery and encourage further preclinical studies in cancer nanomedicine.

**c0054**

**Characterization and investigation of Zinc Oxide Nanomaterials**

[1,a)]Beena. R, [2]Mimi Akash Pateria, [3]Sumita Sengupta
*Department of Applied Physics*
*[1,2]Shri Shankaracharya Technical Campus, Bhilai, Durg, Chhattisgarh, India*
*[3]Shri Shankaracharya Professional University Bhilai, Durg, Chhattisgarh, India*
*a)Email: beenajaykumar@gmail.com*

Nanomaterials and nano dimension composites are attaining a seat in every corner of current scientific world. Numerous nanoparticles are fused via sol gel path. Zinc oxide has countless topography like anti-bacterial, anti-corrosivity, effective photocatalyst etc. This paper reports the material testing and analysis of appropriate sol gel aided preparation of zinc oxide nanoparticles by subjecting samples were subjected to XRD, SEM-EDX, FTIR. The paper also focuses on importance of sol-gel method.

**c0055**

**Role of Dysprosium Doping in Z type Hexaferrite to Enhance Electromagnetic Properties for Antenna Miniaturization**

Anjali Thakur[1]and Mahavir Singh[2]
[1]*Department of Physics, Ramjas College, University of Delhi, Delhi11007*
[2]*Department of Physics, Himachal Pradesh University, Shimla, 171005*
**Email:anjalithakur@ramjas.du.ac.in*

For microwave antenna applications, the magnetic and dielectric properties of hexaferrite ($Co_2Z$) fabricated by sol-gel auto combustion were investigated. Maintaining real permeability (μ) and real permittivity (ε) with controlled electromagnetic losses is a significant difficulty at ultra high frequency range in the communication industry. To meet this need, the current study conducted electromagnetic measurements for magnetic nanoparticles of Dysprosium doped Z-type hexaferrite with compositions $Ba_3Co_2In_{0.1}Dy_xFe_{23.9-x}O_{41}$ (x = 0, 0.05, 0.1, 0.15, 0.2) synthesised by the sol-gel auto combustion soft chemical approach throughout the frequency range of 1-11 GHz. We get excellent permittivity values from average values 6.145 to 9.297 with an increase in doping concentration of Dy and these permittivity values remain almost constant from 1-10 GHz but we are still struggling with the permeability part as it is around 1.5. We get very low magnetic and dielectric loss values which are around 0.2 and 0.28 and 0.02-0.03 respectively. Thus, we obtain the enhanced electromagnetic characteristics of Z-type hexaferrite by doping of Indium and varied concentrations of Dysprosium.

**c0056**

**Temperature-Dependent PL and Optical Study of CIZS Nanoparticles Functionalized with 5-Fluorouracil**

Swati Sharma, Shikshita Jain, S.K. Tripathi[a)]
*Department of Physics, Centre of Advanced Study in Physics, Panjab University, Chandigarh-160014, INDIA.*
*[a)]Corresponding author: surya@pu.ac.in*

In this study, we report the successful conjugation of 5-Fluorouracil (5-FU) to Cu–In–Zn–S (CIZS) quantum dots, thereby developing a nanocarrier system with enhanced optical properties and potential for targeted drug delivery. The 5-FU-conjugated CIZS nanoparticles (NPs) were synthesized at room temperature and characterized using UV-Visible absorption, photoluminescence (PL), and Fourier-transform infrared (FTIR) spectroscopy, and temperature-dependent PL studies. Conjugation with 5-FU was confirmed by a red shift in UV-Visible spectra and the appearance of characteristic vibrational peaks in FTIR, indicates the successful binding through hydrogen bonding and electrostatic interactions. PL intensity showed a moderate quenching upon drug attachment, attributed to charge transfer and surface interaction effects. Temperature-dependent PL studies revealed thermally induced quenching with partial reversibility, suggesting stable binding without compromising the NP's core optical features. These results support the potential of CIZS NPs as a multifunctional platform for simultaneous drug delivery and optical monitoring.

**c0057**

**Mechanical Stability and Elastic Anisotropy in 2D Group III Nitride Monolayers**

Janvi V. Gajjar[1, a] and Debesh R. Roy[1]
[1]*Department of Physics, Sardar Vallabhbhai Patel National Institute of Technology, Ichannath, Surat-395007, Gujarat, India.*
*[a)] Corresponding author: janvigajjar168@yahoo.com*

The mechanical properties of two-dimensional (2D) materials play a pivotal role in determining their reliability and performance in nanoscale devices, especially under strain-induced conditions. Using density functional theory (DFT), we systematically investigate the elastic constants, Young's modulus, and Poisson's ratio of group III nitride monolayers (BN, AlN, GaN, InN) in the

hexagonal phase. Our results reveal their mechanical stability, anisotropic nature, and tunable stiffness, with BN exhibiting the highest rigidity and InN showing maximum incompressibility. These findings provide valuable insights for designing flexible and strain-engineered nanoelectronic applications.

**c0058**

**Visible-Light Driven Photocatalytic Degradation of Antibiotic using Green Synthesized Ce-doped $TiO_2$ Nanoparticles**

Ashwini S. Gadge[1], Anisha Sahu[1], and Dr. R. S. Gedam [a)]
*Department of Physics, Visvesvaraya National Institute of Technology (VNIT), Nagpur,440010*
*[a)]Corresponding author: Rupesh_gedam@rediffmail.com*

The contamination of freshwater with harmful antibiotic pollutants has driven researchers to create new, efficient, and affordable water purification methods and materials. As a result, photocatalysis has emerged as a highly efficient method for addressing environmental remediation. Herein, this work presents the novel green synthesis of Ce-doped $TiO_2$ nanoparticles via the hydrothermal method using *Piper betel* leaves extract. The detailed structural, morphological, and optical properties of synthesized nanoparticles were studied by various characterization techniques, and their photocatalytic activity was tested for the degradation of ciprofloxacin (CIP) under visible light irradiation. The maximum degradation efficiency was found to be 98.25% in 120 minutes of visible light irradiation.

**c0059**

**Tailoring Optical and Structural Properties of Polycarbazole–$TiO_2$ Nanocomposites as an Emissive Layer for OLED Applications**

Gobind Mandal[1], Jayanta Bauri[2], Ram Bilash Choudhary[3] and Satyajit Hazra[4]
*[1,4]Surface Physics & Materials Science, Saha Institute of Nuclear Physics, Bidhannagar, Kolkata-700064, India.*
*[2]Department of Chemistry, Indian Institute of Technology, Bombay-400076, India*
*[3]Nanostructured Composite Materials Laboratory, Indian Institute of Technology (Indian School of Mines), Dhanbad-826004, India.*
**Email: gobindism@gmail.com*

The demand for high-performance Organic light emitting devices (OLEDs) has intensified in recent years, prompting significant research efforts towards the development of advanced emissive materials. Here we report the synthesis and characterization of a novel nanocomposite comprised of polycarbazole (PCZ) and titanium dioxide ($TiO_2$) for application as an emissive material in OLEDs. The resulting nanocomposite exhibits enhanced structural and optical performance, combining the high conductivity of PCZ with the superior electrical properties of $TiO_2$. The formation of PCZ with the correlative change in the nanostructure with the embodiment of $TiO_2$ was confirmed by X-ray diffraction technique (XRD). Irregular tetragonal bipyramidal arrangement of $TiO_2$ was formed over the agglomerated nanospheres of PCZ as confirmed by FESM images. The PL emission spectrum of PCZ-$TiO_2$ nanocomposite showed four emission peaks in the visible spectrum 391 nm, 414 nm, and 440 nm. The reinforcement of $TiO_2$ into PCZ matrix greatly enhanced the PL intensity that refers the more radiative electron-hole recombination which suggested the PCZ-$TiO_2$ nanocomposite could be a potential candidate as emissive layer for OLEDs.

**c0060**

**Controlled Pattern Formation on a Ferrofluid Surface**

Akshat Gupta[1], Rumal Singh[1], Prashant Hitaishi[1], Syed M. Kamil[1], Sajal K. Ghosh[1,*]
[1]*Department of Physics, School of Natural Sciences, Shiv Nadar Institution of Eminence, NH-91, Tehsil Dadri, Gautam Buddha Nagar, Uttar Pradesh-201314, India*
*[*]Corresponding author: sajal.ghosh@snu.edu.in*

Rosensweig instability is the formation of spikes and valleys on a ferrofluid surface under an application of external magnetic field, perpendicular (normal) to the surface of ferrofluid. In this work, the instability was examined by changing the properties of ferrofluid with varying magnetic field. The experiments were conducted using a custom-built experimental setup, comprising a camera, light source, and a sample stage. Beyond a critical magnetic field ($B_c$), applied vertically to a ferrofluid drop, a principal spike form. An increment in the magnetic field results in a rise in its height to a maximum. On further increase of the field, secondary and tertiary spikes are formed around the central spike, conserving the volume of the fluid. The height of the spikes is observed to be dependent on the initial droplet volume and the concentration of magnetic nanoparticles in ferrofluid.

**c0061**

**AI-Enhanced Carbon Nanotube Composite Sensors for Real-Time VOC Detection at Room Temperature**

Rohan Rohilla[1,2], Kinshuk Dasgupta[1,2], Jyoti Prakash[1,2]
*[1]Materials Group, Bhabha Atomic Research Centre, Mumbai-400085*
*[2]Homi Bhabha National Institute, Mumbai-400094*
**Email:jprakash@barc.gov.in*

Volatile organic compounds (VOCs) pose serious health risks, yet conventional detection methods are costly and slow. We present a low-cost chemiresistive sensor using CNT films functionalized with g-$C_3N_4$, CuO, $TiO_2$, $WO_3$, and $V_2O_5$ for rapid, selective VOC detection. AI algorithms accurately classify six VOCs—ethanol, methanol, acetone, toluene, benzene, and hexane—across ppm to ppb levels. Sensors are fabricated via CCVD, acid treatment, dip-coating, and sputtering for uniform, stable performance. The

platform achieves a 2-s minimum response time and a 10 ppb detection limit. Real-time data processing and visualization enable immediate alerts for hazardous VOC levels. Low power consumption and room-temperature operation suit wearable and IoT applications. The modular design supports easy customization for additional target gases. This CNT-AI integration offers a scalable, portable solution for environmental monitoring, industrial safety, and public health protection.

**c0062**

**Unraveling the Structural Evolution of GaAs Nanoribbons into Nanotubes via Ab-initio Simulations**

Anjna Devi[1, a)], Shivani Thakur[3], Bidhi Chand[1], Samiksha Chauhan[2] Neha Thakur[3] Arun Kumar[2,]
[1]*Department of Physics, Government Degree College, Baroh, Kangra, HP, India*
[2]*Department of Physics, Government Degree College, Bilaspur, Bilaspur, HP, India*
[3]*Department of Physics and Materials Science, Jaypee University of Information Technology, Waknaghat, Solan, HP, India*
[a)]*Corresponding author: anjnahpu90@gmail.com*

We study the structure and electronic behavior of non-hydrogenated GaAs nanotubes formed from armchair and zigzag nanoribbons after optimization. The transformation into nanotubes is influenced by their chirality and number of atoms. Our results, similar to earlier studies on hydrogenated nanotubes, show that all GaAs nanotubes have direct band gaps, making them promising for electronic use. Binding energy analysis reveals that armchair nanotubes (AGaAsNT) are more stable than zigzag nanotubes. (ZGaAsNT). The smaller band gaps in zigzag nanotubes make them well suited for sensors, optoelectronics, and advanced nanoelectronic technologies.

**c0063**

**Fluorescence and random lasing studies in Core shell $Fe_2O_3$@$TiO_2$ Nanoparticles dispersed Rhodamine- B solution**

Aneesh Ayyappan and Ashok Vudayagiri
*University of Hyderabad, Gachibowli, Telangana, India-500046*
*ashok_vs@uohyd.ac.in*

This study focuses on regulating the random lasing and fluorescence behavior by employing $Fe_2O_3$@$TiO_2$ core–shell magnetic nanoparticles (MNPs) as scattering centers in a Rhodamine-B dye solution. The samples were characterized using Field emission scanning electron microscopy and UV-Vis absorption spectroscopy in the visible range. Random lasing was excited using the second harmonic (532 nm) of an Nd:YAG laser, and the resulting emission spectra were recorded using a spectrometer. Emission spectra at various MNP concentrations were analyzed, with the $10^{-4}$ M sample exhibiting the strongest emission, suggesting it provides the most effective scattering for enhanced lasing. Measurements were carried out both in the absence and presence of an external magnetic field, with field strengths ranging from 0 to 100 Gauss. The $TiO_2$ shell was found to improve scattering efficiency and boost fluorescence. Additionally, a shift in the emission spectra with increasing magnetic field indicated the tunability of the system through magnetic control.

**c0065**

**Structural, Morphological and Luminescence Properties of Green Synthesized Magnesium Ferrite Nanoparticles**

Vinayakprasanna N. Hegde[1], a, Manju V. V.[1]and Hemaraju B. C.[2]
[1]*Department of Physics, Vidyavardhaka College Engineering, Mysuru-570002, India.*
[2]*Department of Physics, Malnad College of Engineering, Hassan- 573202, India.*
** vinayak.phy@vvce.ac.in*

The present study investigates the synthesis and analysis of magnesium ferrite nanoparticles ($MgFe_2O_4$ NPs) intended for use in opto-electronic devices. The solution combustion method is used to synthesize $MgFe_2O_4$ NPs, resulting in high-purity cubic crystalline phase. The MgFe2O4 NPs exhibits a porous, agglomerated morphology. Density functional theory (DFT) analysis of band structure reveals that conduction band is dispersed, and valance band is dense. Optical analysis revealed a strong absorption peak at ~338 nm, with bandgap energy ranging from 2.2 eV (1.8 eV from DFT). luminescence and chromaticity studies showed that prominent bluish-green luminescence is suitable for lighting and display applications.

**c0066**

**CuO Nanoparticles Confined In KIT-6: Linking Particle Size To Magnetic And Photocatalytic Properties**

Sagnik Mitra[a,b],Adarsh Kumar [a,b],Deepak Tyagi[a,b],Debasis Sen [b,c], Ahin Roy[d], Mayuresh D. Mukadam [b,c], Kaustava Bhattacharyya*[a,b],Avesh Kumar Tyagi *[b]
[a]*Chemistry Division, Bhabha Atomic Research Centre, Mumbai-400 085, India*
[b]*Homi Bhabha National Institute, Mumbai - 400 094, India*
[c]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400 085,India*
[d]*Materials Science Centre, Indian Institute of Technology Kharagpur, West Bengal-721302, India*
**Email: sagnik@barc.gov.in*

Size-dependent variations in material properties, particularly in photocatalytic and magnetic behavior, have long been of significant scientific interest. In this study, CuO nanoparticles were incorporated into mesoporous KIT-6 via a wet impregnation method. Varying the CuO loading resulted in different particle sizes with a narrow size distribution. The resulting materials were characterized using Small-Angle X-ray Scattering (SAXS), X-ray Diffraction (XRD), X-ray Photoelectron Spectroscopy (XPS), High-Resolution Transmission Electron Microscopy (HR-TEM), Scanning Transmission Electron Microscopy (STEM), EELS

mapping, and Electron Paramagnetic Resonance (EPR). The CuO particles were dispersed as clusters within the mesoporous channels. The magnetic and photocatalytic properties of the CuO–KIT-6 (CK) composites were examined as a function of particle size. Photocatalytic degradation experiments using ortho-dichlorobenzene (o-DCB) demonstrated that the CK materials acted as effective photocatalysts, achieving partial degradation of o-DCB. A degradation mechanism, dependent on particle size and influenced by the interplay between magnetic and photocatalytic properties, is proposed.

**c0067**

**Gamma Radiation-Induced Reduction of Graphene Oxide: Nanostructure Evolution and Electric Property Modulation**

Pragati Patil[1,2 a)], Arijit Ghoshal[1,2] RK Mondal[1,2], and KA Dubey[1,2]
[1]*Homi Bhabha National Institute, Mumbai-400094, India.*
[2]*Radiation Technology Development Division, Bhabha Atomic Research Center, Mumbai-400084, India.*
**Email: pragati.patil64@gmail.com*

This study presents a comprehensive investigation of the gamma radiation-induced reduction of graphene oxide (GO) to reduced graphene oxide (rGO), highlighting the impact on nanostructure and dielectric properties. Gamma radiation serves as a clean, chemical-free method to reduce GO via radiolytic generation of solvated electrons and reactive radicals. The extent of reduction was systematically studied at various absorbed doses, ranging from 0 to 10 kGy. Structural evolution was tracked using UV-Vis spectroscopy, transmission electron microscopy (TEM), while electric properties were analyzed across a 4Hz-5MHz frequency range. The results demonstrate a significant decrease in oxygen functionalities, enhanced electrical conductivity.

**c0068**

**Hydrophobicity-Driven Evolution of Interparticle Attraction in Nanoparticle–Pluronic Conjugates**

Sugam Kumar[1,2,*], Debes Ray[1] and Vinod K. Aswal[1, 2]
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085 India*
[2]*Homi Bhabha National Institute, Mumbai 400094, India.*
**Email:sugam@barc.gov.in*

Pluronics are amphiphilic triblock copolymers composed of polyethylene oxide (PEO) and polypropylene oxide (PPO) blocks arranged in a PEO–PPO–PEO manner. By varying the number of PEO and PPO units, Pluronics exhibit different hydrophilic–lipophilic balances (HLB), which determine their relative hydrophobicity or hydrophilicity. These polymers are known to strongly interact with silica nanoparticles, adsorbing onto their surfaces primarily through hydrogen bonding. In this study, we investigate the evolution of attractive interactions among nanoparticle–Pluronic conjugates formed with two Pluronics of distinctly different HLB values: P85 (EO25PO40EO25), which is more hydrophobic, and F88 (EO96PO39EO96), which is more hydrophilic. Our results show that the strength and range of interparticle attraction increase with temperature, driven by the enhanced hydrophobicity of the Pluronic chains. This effect is pronounced for the more hydrophobic P85 but is significantly weaker for the less hydrophobic F88. These findings provide valuable insights into tailoring thermo-responsive soft nano-colloids.

**c0069**

**Phase Evolution, Morphology and Photoluminescence properties of Cr doped $K_3AlF_6$ Nanophosphors: Role of Calcination Temperature**

Rashmi[1] and Sandeep Kumar[1*]
[1]*Department of Physics, Motilal Nehru National Institute of Technology Allahabad, Prayagraj-211004, India*
*Corresponding Author Email: sandeep_kumar@mnnit.ac.in*

This work investigates $K_3AlF_6$:$xCr^{3+}$ ($x$ = 0.005) (KAF:$Cr^{3+}$) for the evolution of structure, morphology, and photoluminescence (PL) properties. KAF is a polymorph possessing monoclinic ($\alpha$), tetragonal ($\beta$), orthorhombic ($\gamma$) and cubic ($\delta$) phase. KAF:$Cr^{3+}$ have been synthesized using coprecipitation method. The as prepared (AP) KAF exhibits $\delta$-cubic phase which remains the same up to 300 $^oC$ and interestingly transform to $\beta$-tetragonal at 500 and 600 $^oC$. The morphological study reveals octahedral shaped particles which gets larger as the calcination temperature increases. Photoluminescence (PL) study shows the enhanced PL intensity peaking around 730 nm in the red region of visible spectrum in case of 300 $^oC$ calcined sample compared to AP sample. Thus, the novel calcined KAF: 0.5at% $Cr^{3+}$ offers promising optical features useful in anti-counterfeiting and other applications like LED fabrication.

**c0070**

**Synthesis, Structural and Spectroscopic Investigation of $Sm^{3+}$ Doped Gadolinium Tungstate and Molybdate**

Mahendra B. Choudhary and Venkatesha R. Hathwar*
*School of Physical and Applied Sciences, Goa University, Taleigao Plateau, Goa 403206*
**Email: vhathwar@unigoa.ac.in*

A series of $Gd_{2-x}(MO_4)_3$: xSm (M= Mo and W) (x= 0.1, 0.2 and 0.3) samples were synthesized by hydrothermal method and characterized by powder X-ray diffraction (PXRD), scanning electron microscopy (SEM), UV-DRS spectroscopy and photoluminescence (PL) spectroscopy. The synthesized phosphor crystalises in pure phase with monoclinic structure. Rietveld refinement results confirms that all the compounds were crystallized under monoclinic system with space group C2/c. SEM reveals that mean particle size ranges between 200 nm to 500 nm. The PL excitation spectrum reveals that the $Gd_{2-x}(MO_4)_3$: xSm (M= Mo

and W) (x= 0.1, 0.2 and 0.3) phosphors can be excited at $\lambda_{exc}$ = 405nm which leads the emission at $\lambda_{emi}$ = 650nm. The Concentration quenching takes place as $Sm^{3+}$ doping concentration increases and this can be attributed to multipole-multipole interaction.

**c0071**

**Study of Optical, Magnetic and Dielectric Properties of ZnCo-ferrite Nanoparticles**

Anna Rose Binu[1], Tweja K V[1], Malavika A S[1], Subasa C. Sahoo[1*]
[1]*Department of Physics, Central University of Kerala, Periya, Kasaragod, Kerala 671325, India*
**subasa.cs@gmail.com*

$Co_{0.8}Zn_{0.2}Fe_2O_4$ nanoparticles were prepared by the sol-gel auto-combustion method and were annealed at 900 °C. Single-phase cubic spinel structure was confirmed by XRD, with crystallite size of 26.5 nm. FTIR analysis established metal–oxygen vibration corresponding to the spinel structure in the sample. UV–Vis spectroscopy showed a direct band gap of 1.38 eV. The spontaneous magnetization value of 77.62 emu/g was observed at 300 K and it was enhanced to 91.8 emu/g at 10K with very high coercivity of 1.64kOe. Dielectric characterization was done with frequency and at different temperatures for possible application at high frequencies.

**c0072**

**Structural, Vibrational, and Electrical Characteristics of Pyrochlore Structured Ce-Doped $La_2Sn_2O_7$**

Abhijith Sreekumar[1] and P. Thangadurai[1], *
[1]*Centre for Nanoscience and Technology, Pondicherry University, Kalapet, Puducherry- 605014, India*
**Corresponding author: thangaduraip.nst@pondiuni.edu.in / thangadurai.p@gmail.com*

Nanocrystalline $La_2Sn_2O_7$ (LSO) and Ce-doped $La_2Sn_{2-x}Ce_xO_7$ (x = 0.01, 0.05) were synthesised via co-precipitation method followed by calcination at 1000 °C. XRD analysis confirmed a single-phase cubic pyrochlore structure with ~41–45 nm crystallite size. Raman spectroscopy showed characteristic modes of the pyrochlore lattice, with Ce doping causing slight redshift and peak broadening due to local structural distortions. XPS analysis verified the oxidation states and successful Ce incorporation. Impedance spectroscopy revealed a non-Debye-type ionic conduction, with activation energies of 0.59 eV (undoped), 0.65 eV (1% Ce), and 0.49 eV (5% Ce). Ce doping improved conductivity while preserving structural integrity, indicating potential for high-temperature electrochemical applications.

**c0073**

**Studies on Structural and Electrical Properties of ZnO-Based $LaMnO_3$ Nanocomposite**

Keval Gadani[1,a)], Indrajitsinh Bihola[2], C.M. Panchasara[2], Himitri Trivedi[2], Bharavi Hirpara[2], P.S. Solanki[2], N.A. Shah[2]
[1] *Centre of Education, Indian Institute of Teacher Education (IITE), Gandhinagar – 382 016, India*
[2] *Department of Physics, Saurashtra University, Rajkot, 360005, Gujarat, India*
**Email: kjgadani@gmail.com*

Structural, microstructural and electrical properties of sol–gel grown ZnO nanoparticles, LaMnO3 (LMO) nanoparticles and ZnO based LaMnO3 (LMO50) nanocomposites have been studied. Nanocomposite was prepared by addition of ZnO content (50% wt %) in LMO manganite. The θ–2θ X–ray diffraction (XRD) measurement reveals the single-phase nature without any detectable impurity. Rietveld refinements have been performed using FULLPROF software to verify the structural phase purity for all three samples. Transmission electron microscopy (TEM) images provide modification in the grain size and particle size for ZnO nanoparticles, LMO nanoparticles and LMO50 nanocomposite. Dielectric behavior has been understood in the context of cole–cole relaxation model fits very well throughout the frequency range studied. Variation in a.c. conductivity has been discussed on the basis of Jonscher's universal power law. Power law fits suggest that charge conduction becomes possible through the correlated barrier hopping (CBH) mechanism.

**c0074**

**Levels of Polaron in Metal Halide Perovskite Quantum Dots with Parabolic and Gaussian Potentials**

Thara Angoth[1, a)], Anusha Kachu[1], Aalu Boda[1, b)]
[1]Department of Physics, National Institute of Technology, Warangal-506004, Telangana, India.
[a)] Corresponding author: at23phr2r02@student.nitw.ac.in
[b)] abdop@nitw.ac.in

In this work, we theoretically investigate three metal halide perovskite quantum dot ($MAPbBr_3$) with both parabolic and Gaussian confinement potentials. Using a unitary transformation and the Pekar-type variational method, we calculate the polaron ground and first excited state energies arising from electron–phonon interactions. Transition energies are also evaluated. The results reveal that Gaussian confinement leads to stronger localization and lower energy states. The type of potential has a significant influence on polaron characteristics. This work contributes to the understanding of polarons in perovskite nanostructures for optoelectronic applications.

**c0075**

**Electrochemical Performance Of Hybrid Perovskite $CH_5N_2PbI_3$: A Potential Electrode For Energy Storage**

Ashik Ikbal[1], Arijit Ghosal[1], Payal Sengupta[2], Saheli Ghosh[1] and Ruma Ray[1, a)]
[1] *Department of Physics, Jadavpur Unniversity,188 Raja SC Mallick Road, Jadavpur, Kolkata 700032, India*

[2]*School of materials Science, Indian Association for the Cultivation of Science, Kolkata-700032*
**Email address: juphyruma@gmail.com*
Hybrid perovskites have emerged as promising materials for energy storage applications due to their high ionic-electronic conductivity and excellent electrochemical stability. They are also suitable for photo-rechargeable supercapacitors i.e., it can convert solar energy into electrical energy and store it simultaneously, offering a promising avenue for sustainable energy solutions. This study involves with the synthesis, structural characterization and investigation of electrochemical performance of formamidinium lead iodide ($CH_5N_2PbI_3$) hence named as FAPbI and highlights its charge storage mechanisms. Electrochemical analysis using cyclic voltammetry (CV) and galvanostatic charge–discharge (GCD) in a three-electrode setup revealed excellent specific capacitances of 127 F/g at 5 mV $s^{-1}$ and 121 F/g at 4 A $g^{-1}$ respectively. Detail analysis of the experimental results distinguishes the capacitive and diffusive contribution towards the charge storage mechanism.

**c0076**

**Nanoparticle-Fuel for Smoother Engines**

Anvisha Patwa and Nehal Maheshwari
[1]*School of Technology Management & Engineering, SVKM`s NMIMS, Indore-453112*
*ANVISHA.PATWA065@nmims.in*
This research investigates the impact of incorporating titanium dioxide ($TiO_2$) and copper oxide (CuO) nanoparticles into conventional fuel on engine-induced and hand–arm driver vibrations. Vibrations transmitted through the vehicle can lead to driver discomfort and long-term physical strain. To assess the effects, fuels were blended with varying nanoparticle concentrations (0, 50, 100, and 150 ppm) and tested at different engine speeds (1000, 2000, and 3000 rpm). Key parameters such as fuel viscosity, density, calorific value, and engine brake power were measured. The results revealed that nanoparticle-enhanced fuels improved engine performance and significantly reduced vibration levels, particularly at 3000 rpm. At a concentration of 150 ppm, CuO and $TiO_2$ nanoparticles reduced overall engine vibrations by over 30% and nearly 29%, respectively. Notably, only 8–10% of these vibrations were transmitted to the steering wheel, and CuO demonstrated a greater reduction in this transfer. These findings suggest that nanoparticle additives in fuel can enhance driving comfort and reduce mechanical stress on vehicle components.

**c0077**

**Transition Metal Induced Tuning of Photocatalytic Activity of Multiferroic $BiFeO_3$ and $BiMnO_3$**

Arijit Ghosal[1], Ashik Ikbal[1], Payal Sengupta[2], Saheli Ghosh[1], Ruma Ray[1,*]
[1]*Department of Physics, Jadavpur University, Kolkata 700032, India*
[2]*School of Materials Science, Indian association for the Cultivation of Science (IACS), Kolkata 700032, India*
**Email: juphyruma@gmail.com*
The rapid growth of dye-intensive industries has led to the accumulation of persistent dyes in aquatic systems, demanding efficient treatment solutions. Visible-light-activated semiconductors enable pollutant abatement. This work explores photocatalytic activity of $BiTMO_3$ (TM= Fe, Mn) Structural characterizations of $BiTMO_3$ were performed by XRD which infer, its crystallite sizes 26.4 nm and 35.2 nm, respectively. UV-Vis spectroscopy inferred its band gap as 2.51 eV and 2.95 eV for $BiFeO_3$ and $BiMnO_3$, respectively. Photocatalytic activity of $BiFeO_3$ and $BiMnO_3$ are found to be 71.0 % and 73.5 %, respectively for 150 min irradiation of visible light. It is noteworthy that although $BiFeO_3$ has a smaller particle size and a narrower optical band gap compared to $BiMnO_3$, the presence of the transition metal Mn makes $BiMnO_3$ a more effective agent for dye degradation.

**c0079**

**Synthesis and characterization of various size gold nanoparticles for catalytic activity in sealed-off $CO_2$ laser**

Avantika Gautam[1,2 a)], Shweta Verma[1], B Tirumala Rao[1], Rashmi Singh[3], Rajiv Kumar Yadav[1], L. B. Rana[1], Sunil Verma[2,3] and Manoj Kumar[1]
[1]*$CO_2$ Laser Technology Section, Raja Ramanna Centre for Advanced Technology, Indore, 452013, Madhya Pradesh, India*
[2]*Homi Bhabha National Institute, BARC Training School Complex, Anushakti Nagar, Mumbai, 400094, India*
[3]*Photonic Materials Technology Section, Raja Ramanna Centre for Advanced Technology, Indore, 452013, Madhya Pradesh, India*
**Email: avantika@rrcat.gov.in*
Commercial glass tube sealed off $CO_2$ laser use gold nanoparticles (Au NPs) coating as catalyst for maintaining constant $CO_2$ lasing molecules by recombining CO and $O_2$, which are produced due to dissociation of $CO_2$ under discharge conditions. In this study, Au NPs of various sizes were synthesized and characterized by UV-Visible spectroscopy. These nanoparticles were subsequently deposited on to silicon substrate via drop casting and thoroughly characterized using scanning electron microscopy (SEM) and X-ray diffraction (XRD) to evaluate their morphology and crystallinity. Based on these characterizations, Au NPs with sizes below 30 nm was then deposited onto glass substrate and annealed at 200°C. Characterization of Au NPs deposited on glass substrate revealed that the deposited nanoparticles were approximately five times smaller than those used in commercial tubes. A reduction in size is expected to enhance catalytic efficiency and extend the operational lifetime of the laser. Hence, these sub-30 nm Au NPs were subsequently coated onto the inner surface of glass tubes for potential application in sealed-off $CO_2$ laser.

**c0081**

**Nanoengineering Portland Cement Mortars With Borophene Quantum Dots: A Route To Enhanced Strength And Microstructural Optimization**

H.J. Yashwanth[1*], M. Madhukar Naik[2], K Ranjitha[1], H B Shivaprasadh[1], Hitha D Shetty[1], K N Narasimha Murthy[3]
*[1]Nitte Meenakshi Institute of Technology, Nitte(Deemed to be university) Bengaluru 560107, India*
*[2]Department of Chemistry, BMS Institute of Technology & management, Bengaluru 560107, India*
*[3]Department of Physics, Government First grade college, Bangalore, 560064, India*
**Corresponding author: yashwanthhj95534@gmail.com*
Borophene, a monolayer of boron atoms and the lightest elements Dirac material, has developed as a highly promising two-dimensional (2D) nanomaterial due to its exceptional structural, mechanical and electrical properties. Among its derivatives, borophene quantum dots (BQDs) have gained attention as a novel zero-dimensional material with significant potential in advanced composite applications. This study investigates the impact of BQDs on the mechanical and microstructural properties of cement mortar composites. Results demonstrate a notable enhancement in compressive strength at 28 days with the incorporation of BQDs. Microstructural analysis further reveals the development of a denser cement matrix, attributed to the presence of BQDs. These findings suggest that BQDs are a promising nanomaterial for reinforcing cementitious systems, offering improved performance and durability.

**c0082**

**Investigating Pyrochlore – Fluorite Structural Conundrum in co-doped Rare Earth Zirconates**

Raghavendra K. G[1*], M Vidya[1], Saideep Shireesh Bhat[2], Gurumurthy S. C[2]
*[1]Department of Physics, Manipal Institute of Technology, MAHE, Manipal – 576104, Karnataka, India*
*[2]Nano and Functional Materials Lab (NFML), Department of Physics, Manipal Institute of Technology, MAHE, Manipal – 576104, Karnataka, India*
**Email: raghavendra.kg@manipal.edu*
The present study examines the structural evolution of $Gd^{3+}$ and $Ce^{4+}$ co-doped lanthanum zirconates, synthesized via co-precipitation. Phase transformations between 700–1300 °C were analyzed using X-ray diffraction and Raman spectroscopy. The La-rich composition transitioned from a disordered to an ordered pyrochlore phase, evidenced by the emergence of superlattice reflections. In contrast, the Gd-rich sample stabilized in a defect fluorite structure without superlattice peaks, though Raman spectra indicated weakly ordered pyrochlore microdomains, suggesting phase coexistence. TEM diffraction analysis confirmed these findings. Structural changes were correlated with variations in the average cation radius ratio from $Gd^{3+}$ and $Ce^{4+}$ incorporation. Williamson–Hall analysis showed both samples retained nanostructures with crystallite sizes under 100 nm, and SEM observations supported the structural stability.

**c0083**

**Photon Induced Responses On Electrical Properties Of Nanocrystalline Porous Silicon**

Pardhu Yella[1], V S Vendamani[2]
*[1]Department of Physics and Chemistry, Mahatma Gandhi Institute of Technology, Gandipet, Hyderabad 500075, India.*
*[2]School of Physics, University of Hyderabad, Hyderabad 500046, Telangana, India.*
**Email: pardhuyella_phy@mgit.ac.in*
We report a successful formation of sponge like nanocrystalline porous silicon by anodic etching of c-Si. The porosity of porous silicon (pSi) layers was tuned by varying the applied current density during etching process. Photon induced responses on electrical behavior was extracted from current-voltage (I-V) characteristics. We have observed increased current under illumination of light, which is due to photo induced electron excitation in the material. A linear relation between number photons absorbed per second and generated current has been observed. This states that the observed changes in the electrical properties are based on single photon absorption. This study concluded that pSi is one of the effective materials to construct silicon compatible photo detectors with effective cost.

**c0084**

**Hot-injection Based Synthesis and Characterization of Lead-free Cu-Ag-Bi-I Pnictohalide Nanocrystals (NCs)**

Krishnendu Karmakar[1], Chayan Das[1], Arindam Biswas [2,3], Arup K. Rath[2,3], Satyajit Sahu[1a)]
*[1]Department of Physics, Indian Institute of Technology Jodhpur, Jodhpur 342030, India*
*[2]CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pune 411008, India*
*[3]Academy of Scientific and Innovative Research, Ghaziabad, 201002, India*
*email: satyajit@iitj.ac.in*
Solution-processed lead halide perovskites have garnered attention in recent years. Nowadays, research is being conducted to find a suitable alternative for lead, which is poisonous, unstable, and harmful to the environment. Due to their low toxicity and diverse structural dimensions, Pb-free perovskite-inspired materials (PIM) like copper or silver pnictohalides ($A_x$ $B_y$ $X_{x+3y}$) like $CuBiI_4$, $Cu_2BiI_5$, $Cu_2AgBiI_6$, and $Ag_3BiI_6$, are becoming popular for optoelectronic and photocatalytic applications. Hot Injection synthesis of Cu-Ag-Bi-I nanocrystals (NCs) is described here. As synthesised Cu-Ag-Bi-I NCs crystal structure and characteristics were examined. The trigonal structure of Cu-Ag-Bi-I NCs with space group R3m was disclosed by X-ray diffraction. Raman vibrational spectroscopy is also used for Cu-Ag-Bi-I nanocrystals. A detailed investigation of Cu-Ag-Bi-I nanocrystal composition and chemical states is also provided. According to UV-Vis spectroscopy, the Cu-Ag-Bi-I perovskite NCs have a direct band gap. The study on Cu-Ag-Bi-I NCs reveals potential as a lead-replacement material for various Optoelectronics, RRAM (Resistive random access memory), photodetectors, and solar energy harvesting applications.

**c0085**

**Effect of Antimony (Sb) doping on the structural and optical Properties of $Cs_2CuBiCl_6$ Halide Double Perovskite**

Manoj Bora* and Mahananda Baro
Department of Physics, Assam University, Silchar, 788011, India
**Email:manojbora27@gmail.com*

Lead-free halide double perovskites have emerged as promising substitute to lead-based materials for optoelectronic applications because they are more stable and less toxic. In this study, we examined the effect of antimony ($Sb^{3+}$) doping on the structural and optical characteristics of the lead-free double perovskite Cs2CuBiCl6. We have synthesized a series of Sb-doped compounds with the general formula Cs2CuBi1-xSbxCl6 (x = 0.0, 0.1, 0.2, 0.3) using a solution-based method under ambient conditions. X-ray diffraction (XRD) analysis confirmed the formation of a double perovskite structure for all compositions. There are slight peak shifts in the XRD spectra that indicate lattice contraction due to $Sb^{3+}$ incorporation. Additionally, samples are characterized using UV–Vis and photoluminescence (PL) spectroscopy. UV-Vis spectroscopy showed a systematic narrowing of the band gap as Sb3+ content increased, which may be attributed to the alteration in the electronic structure caused by doping. We demonstrated that Sb3+ substitution effectively modifies the structural and optical properties of Cs2CuBiCl6, highlighting its potential in environmentally friendly optoelectronic devices.

**c0086**

**Enhanced Electrical and Optical Properties of CuO-MWCNT Nanocomposite Synthesized via Ultrasonic Method**

Hetal Gohil[1], Krina Ramani[1], V.R. Chandegara[1], H.M. Oza[1], Sangita Chavda[1], H.C. Kamdar[1], P.S. Solanki[1], A.D. Joshi[2], Davit Dhruv[1], N.A. Shah[1], R.K. Trivedi[3,4, *)]
*[1]Department of Physics, Saurashtra University, Rajkot, 360 005, Gujarat, India*
*[2]Department of Nanoscience and Advanced Materials, Saurashtra University, Rajkot, 360 005, Gujarat, India*
*[3]H & H. B. Kotak Institute of Science (Saurashtra University), Rajkot, 360 001, Gujarat, India*
*[4]Bahauddin Science College (Bhakta Kavi Narsinh Mehta University), Junagadh,362001, Gujarat, India*
**Email: rupalktrivedi@yahoo.com*

The current work focuses on the CuO/MWCNT nano composites. CuO nanoparticles were prepared using sol-gel method, while the MWCNT was taken readily at the nanometer scale. Ultrasonic approach was used to prepare the CuO/MWCNT nanocomposite in different (1%, 3%, and 5%) nano composites by adding varying amounts of MWCNT. XRD measurements were taken in θ-2θ mode which confirmed the monoclinic crystal structure and the particular space group is C2/c. FESEM was carried out to examine the microstructural characteristics and showcase the presence of MWCNT particles in the synthesized nanocomposites. The UV-Visible spectroscopy measurement was carried out to determine the energy band gap of CuO and composite materials. Analysis showed that when MWCNT concentration rises, the energy band decreases. Dielectric behavior was studied using the Agilent make LCR meter in the frequency range of 20 Hz to 2 MHz. The behavior of dielectric constant, impedance and ac conductivity were examined in relation to the conducting MWCNT and the function of CuO semiconductor nature.

**c0087**

**$MoS_2$ as a Multifunctional Material for Efficiency Enhancement in Thin-Film GaAs Solar Cells**

Jagmeet Singh Sekhon[1, a)] Lakhveer Singh Khana[2] and Gurjit Singh[1]
*[1]Department of Physics, Govind National College Narangwal, Ludhiana, Punjab 141203*
*[2]Department of Mechanical & Production Engineering, Guru Nanak Dev Engineering College, Ludhiana, Punjab*
**Email:jagmeetsekhon@ymail.com*

This study investigates a synergistic approach to enhance the performance of Gallium Arsenide (GaAs) semiconductor devices by integrating molybdenum disulfide ($MoS_2$) nanostructures. The optical analysis carried out by Finite Difference Time Domain revealed that the $MoS_2$ nanoparticles induce a strong Localized Surface Plasmon Resonance (LSPR) effect, significantly boosting light absorption in the 550-750 nm wavelength range in comparison to a continuous $MoS_2$ layer. This plasmonic enhancement effectively complements the intrinsic absorption of GaAs, creating a broadened and intensified absorption profile. The optical improvements directly translate into superior electrical performance, with the short-circuit current density (Jsc) being highest in the configuration combining a continuous $MoS_2$ layer with nanoparticles. We found a direct correlation between enhanced light absorption and increased charge carrier generation. After recursive analysis, the optimal geometrical properties for the best performance within the solar spectrum were determined to be a nanoparticle radius of 40 nm, a period of 100 nm, and an $MoS_2$ layer thickness of 20 nm. This approach paves the way for developing more efficient, high-performance next-generation optoelectronic devices.

**c0088**

**Large Area Fabrication Of Two-Dimensional $PtX_2$ (X=S, Se) Heterostructures For Broadband Photodetector Studies**

Gaurav Bassi, Mukesh Kumar
*Functional and Renewable Energy Materials Laboratory, Department of Physics, Indian Institute of Technology Ropar, Rupnagar, Punjab-140001, India*
*gaurav.19phz0005@iitrpr.ac.in*

Photodetectors are optoelectronic devices that convert light signals into electrical signals and are used to detect a range of the electromagnetic spectrum. My thesis aims to develop $PtX_2$ (X=S, Se) heterostructure-based broadband photodetectors with high performance in the near-infrared (NIR) region. Broadband photodetectors have multiple applications in optical communication, defense security, environmental monitoring, and medical imaging. Two-dimensional (2D) materials, especially group-10 transition metal dichalcogenides (TMDC), $PtX_2$ are highlighted for their distinct properties including narrow band gap range, high carrier mobility, and good ambient stability, required to fabricate high-performance broadband photodetectors. The thesis achieved multiple goals including the large area and controlled growth of $PtS_2$ film by thermally assisted conversion (TAC) method where pre coated Pt film are sulfurized in chemical vapor deposition (CVD). The various growth parameters such as sulfur amount, Pt thickness and carrier gas flow rate are optimized to achieved the high quality $PtS_2$ film on different substrates ($SiO_2$/Si, Si, sapphire and mica). Next, various $PtX_2$ heterostructures including $PtS_2/MoS_2$ (2D-2D), $PtS_{2-x}/Ga_2O_3$ (2D-3D) and $PtSe_2/MoS_2$ based broadband photodetectors with best response in the NIR region are fabricated. Moreover, using X-ray photoelectron spectroscopy (XPS) detailed interface study of the heterojunction including their band alignment and carrier transport mechanism is also carried out. Therefore this work may help to grown large area growth of $PtX_2$ and their heterostructure for future optoelectronics applications.

**c0089**

**ZnS-$Bi_2O_3$ Nanocomposite: An Efficient Material For Environmental Remediation**

Saswata Sahoo [1], N. R. Panda[2], Sangram K. Sahu[1], A. Meher[1], and Dojalisa Sahu[1*]
[1]*School of Applied Sciences, Centurion University of Technology and Management, Odisha, India*
[2]*School of Basic Sciences, Indian Institute of Technology Bhubaneswar, Bhubaneswar, Odisha, India*
**Email: dojalisa.sahu@cutm.ac.in*

ZnS-$Bi_2O_3$ nanocomposite was successfully synthesized using an ultrasound-assisted wet chemical method, aiming to explore its potential for environmental remediation. The structural properties of the composite were characterized using X-ray diffraction (XRD) spectroscopy, confirming the formation of a heterostructured nanocomposite with good crystallinity. FESEM analysis revealed two distinct particle distributions, with smaller ZnS nanoparticles anchored onto larger $Bi_2O_3$ grains. Vibrational properties involving Zn–S and Bi–O bonding features were verified from Fourier-transform infrared (FTIR) study. The photocatalytic performance was evaluated by the degradation of Methylene Blue (MB) dye under UV-visible light irradiation. UV-Vis absorption studies of the dye solutions revealed significant reduction in absorbance, indicating efficient degradation of 84.01%. Kinetic analysis showed that the dye degradation followed pseudo-first-order reaction kinetics. The enhanced photocatalytic activity is attributed to the synergistic effect between ZnS and $Bi_2O_3$, which promotes charge separation and increases active sites. These findings demonstrate that ZnS-$Bi_2O_3$ nanocomposite is a promising material for wastewater treatment application involving organic dyes.

**c0090**

**A Clean Method For Graphene Oxide Modification Toward Biosensing Applications**

Sampa Sutradhar[1,2, a)], Srinibas Satapathy[1,2, b)], S. Raj Mohan [1], Bhumika Sharma[1], Pratik Deshmukh[1,2], Shovan Kumar Majumder[1,2]
[1] *Laser Biomedical Applications Division, Raja Ramanna Centre for Advanced Technology, Indore-452013*
[2]*Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai-400094, India.*
*Email: sampasutradhar@rrcat.gov.in, srinu73@rrcat.gov.in*

Exceptional electrical, optical, chemical and mechanical properties of Graphene and its derivatives, like graphene oxide (GO) and reduced graphene oxide (r-GO), have attracted significant interest in the fields of nanoscience and nanotechnology. For the successful application of graphene and its derivatives, it is indispensable to control the content of this material in production, state of aggregation, aspect ratio etc., which can be achieved through optimizing the synthesis parameters. Synthesizing graphene on a large scale with minimum defects is one of the key challenges. Commonly employed method for achieving graphene like structure with $sp^2$ hybridized carbon is the reduction of GO. In this work, GO is synthesized using modified Hummer's method and reduced further to r-GO using laser irradiation. Chemical, optical and electrical properties of synthesized GO and r-GO were investigated to understand the changes in characteristics of r-GO with reduction rate. Reduction in the defects and the concomitant enhancement in the electrical conductivity assert the suitability of synthesized r-GO for diverse applications.

**c0092**

**Magneto-Structural and Rheological Analysis of Copper Ferrite Ferrofluid in Paraffin Oil**

[1]Nisha Gautam and [2]Rajender Singh
[1]Department of Physics, *Anurag University, Hyderabad-500088, Telangana*
[2]*School of Physics, University of Hyderabad, Hyderabad-500046, Telanagna*
*Email:nishagautam.physics@anurag.edu.in, rsinghsp@gmail.com*

In this paper we have synthesized the $CuFe_2O_4$ using the co-precipitation method. These nanoparticles were coated with oleic acid (1:0.5:1) and homogeneously dispersed in paraffin oil to obtain stable ferrofluid. The X-ray diffraction (XRD) confirmed the single phase with space group Fd-3m. Transmission electron microscopy (TEM) showed the spherical shape. The Vibrating Sample magnetometer (VSM) for magnetic measurements indicated soft magnetic behavior negligible coercivity and saturation magnetization 23 emu/g at 300K. The magneto viscosity of the ferrofluids were explored under applied magnetic fields, revealing

a significant field-dependent increase in viscosity. In magneto viscosity curve the formation of chain-like particle structures aligned with the magnetic field. The study provides valuable insights into the structure–property relationships in $CuFe_2O_4$based ferrofluids and underscores their potential for use in magnetically controlled systems such as dampers, sensors, and biomedical devices.

**c0094**

**Effect of reducing agents on properties of hydrothermally synthesized ZnTe nanomaterials**

Shivaji M Sonawane[1, 2],Jyoti Deshmukh[2],Maruti Salve[2],Priyanka Londhe[2],Shweta Chaure[2, 3] and Nandu Chaure[2, a)]
[1]*Department of Physics, Bharatiya Jain Sanghatana's A. S. & C. College, Pune 412 207, India.*
[2]*Electrochemical Laboratory, Department of Physics, Savitribai Phule Pune University, Pune-411007, India.*
[3]*Department of Physics, COEP Technological University, Pune 411 005, India.*
[a)]*Corresponding author: nchaure.uop@gmail.com*

Zinc telluride (ZnTe) nanomaterials have significant attention for their potential applications in optoelectronics application due to their direct bandgap and high electron mobility. This study investigates the influence of reducing agents, hydrazine hydrate ($N_2H_4 \cdot H_2O$) and sodium borohydride ($NaBH_4$), on the hydrothermal synthesis of ZnTe nanomaterials. The synthesized nanomaterials were characterized using UV-Visible spectroscopy, X-ray diffraction (XRD), and scanning electron microscopy (SEM). The results reveal that the choice of reducing agent significantly affects the crystallite size, morphology, optical bandgap, and surface chemistry of ZnTe nanomaterials. Hydrazine hydrate promotes the formation of smaller, spherical nanoparticles with a bandgap of ~2.25 eV, while sodium borohydride yields larger, rod-like structures with a slightly reduced bandgap of ~2.15 eV. XRD confirms a cubic zincblende structure for both, with varying degrees of crystallinity. SEM and EDS revels morphological differences and elemental purity. These findings underscore the role of reducing agents in tailoring ZnTe nanomaterials for specific applications, offering insights into optimizing synthesis protocols for enhanced optoelectronic properties.

**c0096**

**Tuning Optical Properties of Photonic Crystals Using silver nanoparticles**

A. Vignesh[a)], M. Saraswati and R. G. Joshi
*Materials Science Group, Indira Gandhi Centre for Atomic Research, A CI of Homi Bhabha National Institute, Kalpakkam 603102, India*
[a)] *Corresponding author: vignesh@igcar.gov.in*

We study here an effect of addition of silver nanoparticles on optical properties of self-assembled photonic crystals. The photonic crystals of monodisperse polystyrene particles have been prepared which shows photonic band at ~490nm. Upon addition of the silver nanoparticles, the photonic band exhibits blue shift (i.e. shifts to lower wavelengths) as well as it becomes more stronger (reflectance peak height increases). Blue shift and reflectance peak height continues to increase upto certain silver nanoparticle concentration, beyond which both remains constant. These changes in the photonic band with addition of silver nanoparticles are explained in terms of variation of effective refractive index and index contrast of photonic crystal upon addition of silver nanoparticles.

**c0097**

**Tuning The Electronic And Magnetic Properties Of Graphullerene Via Pd, Y, And Mg Doping: A DFT Study**

Samiksha Chauhan[1a)], Satish Thakur[1], Reena Kumari[1], Rajendra Adhikari[2], Arun Kumar[1]
[1a)] *Govt. College Bilaspur, Himachal Pradesh, India, 174001.*
[2]*Department of Physics, Kathmandu University, Dhulikhel, Nepal.*
[a)]*Email:chauhansamiksha557@gmail.com*

We exploit the electronic and magnetic properties of pristine and doped graphullerene (GF) with Mg, Y and Pd. Here we observe highest magnetic moment 2.0$\mu_B$, in GF@Mg due to the structure distortion. On the other hand, energy band gap of GF@Y increased as compare to the Mg doped in case of spin-up and opposite trend was seen for spin-down. Further Pd doping keeps the material non-magnetic. Moreover, in case of Y or Mg doping first nearest neighbor are contributing most in magnetic moment as compare second and third nearest neighbor. These magnetic and electronic characteristics are very applicable to next-generation technologies. Due to GF@Mg large magnetic moment, it holds promise for high density magnetic storage and spintronics, where the magnetic state can be used to incode information.

**c0098**

**Ammonia Dehydrogenation on Nickel Clusters**

Vaibhav Chauhan,[1,a] Chaithanya Purushottam Bhat,[2] Varun Vinayak Deshpande,[1,3] Debashis Bandyopadhyay,[2] and Soumen Bhattacharyya[1,3]
[1]*Atomic & Molecular Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400 085, India.*
[2]*Physics Department, Birla Institute of Technology and Science, Pilani 333031, Rajasthan, India*
[3]*Homi Bhabha National Institute, Anushaktinagar, Mumbai 400 094, India.*
[a]*Corresponding author: vibhu9494@gmail.com*

Cationic nickel clusters show a unique reactivity toward ammonia, producing stable $H_2$-bound species not observed in their neutral counterparts. Using TOF mass spectrometry and DFT calculations, we uncover that hydrogen evolution is energetically feasible only via co-adsorption of two $NH_3$ molecules, with $Ni_3^+$ being the most favorable catalyst. Cooling the cluster source amplifies $H_2$

attachment, highlighting temperature-dependent reactivity. These findings reveal a charge- and size-specific pathway for ammonia activation and hydrogen release in nickel nanoclusters.

**c0099**

**Dielectric Studies of Cobalt Substituted Lithium Ferrite**

Parul Sharma[1, a)] Palika[1], Preeti Thakur[2] and Atul Thakur[2]
[1]*Department ofPhysics ,Bahra University, 173232, Solan, Himachal Pradesh*
[2]*Amity University, Gurgaon, Haryana.*
[a)] *sharma.parul379@gmail.com*

Lithium ferrites with inverse spinel structure have potential applications in microwave devices and magnetic recording due to their high Curie temperature and magnetization. This study investigates the effect of cobalt substitution on the dielectric and magnetic properties of Li0.5CoxFe2.5-xO4 ferrites. The results show that dielectric loss decreases with increasing frequency, while permeability exhibits dispersion at lower frequencies. Magnetic loss decreases with increasing frequency, and dielectric constant is high at low frequencies. The study suggests that these ferrites have potential applications in magnetic devices, particularly in frequency ranges where permeability is constant. The addition of cobalt ions influences the magnetic loss behavior, making it suitable for specific applications.

**c0100**

**A Computational Study of bg-$C_3N_4$: From Monolayer to Nanoflake**

Bharti Thakur[1,a)], Satish Kumar[1], Ritika Negi[1], Chet Ram[1], Samar Kapila[1], Arun Kumar[1]
[1]*Govt. College Bilaspur, Himachal Pradesh, India, 174001*
[a)]*Corresponding author: bharti7thakur@gmail.com*

We investigate the electronic and magnetic properties of triangular and disk shaped nanoflakes derived from buckled graphitic carbon nitride(bg-$C_3N_4$) using first principle calculations. While the monolayer is nonmagnetic, nanoflakes exhibits geometry-dependent magnetism and band gap modulation. We find out that triangular flakes become magnetic and have smaller band gap, while disk shaped flakes show strong spin asymmetry. The magnetism mainly contributed from edge atoms, and its distribution depends on the flake's geometry. These result shows that by simply changing the shape of bg-$C_3N_4$ nanostructure, we can tune its properties for future spintronics and optoelectronic technologies.

**c0101**

**Tailoring Nonlinear Optical Characteristics in Lanthanum Nickelate Nanoparticles via Zn Doping**

Shija K [1,2] , Muhammed Swalihu P M[3,4], Nandana P[2], N E Rajeevan[2,a]
[1]*Department of Physics, Farook College, Calicut-673632, Kerala, India*
[2]*Department of Physics, Providence Women's College, Calicut-673009, Kerala, India*
[3]*Department of Physics, Catholicate College, Pathanamthitta – 689645, Kerala, India*
[4]*International and Interuniversity Center for Nanoscience and Nanotechnology, Mahatma Gandhi University, Kottayam – 686560, Kerala, India*
**Email: rajeevneclt@gmail.com*

Pristine $LaNiO_3$ and Zn doped $LaNiO_3$ nanostructures have been synthesized using the PVA assisted sol-gel method. This work focuses on determining and enhancing nonlinear optical behaviours, while also identifying these materials as suitable candidates for optical limiting applications. The synthesized nanomaterial was characterized using X-Ray Diffraction (XRD). The energy band gap was calculated from the absorbance spectra which shows decreasing trend due to doping. The Open aperture (OA) Z-scan experiment demonstrated reverse saturable absorption (RSA) resulting from two-photon absorption (2PA). A notable enhancement in the nonlinear absorption coefficient (β) for the doped sample in contrast to the undoped sample, suggesting promising applications in optical limiting and laser protection.

**c0102**

**Structural Comparison of Bulk Cobalt and Carbon Encapsulated Cobalt Nanopowder using 59Co NMR**

[1]Arunkumar S M, [1]Thipperudrappa J, [2]Manjunatha M*,
[1]*Department of Studies in Physics, Vijayanagara Shri Krishnadevaraya University, Ballari, India**
[2]*Department of Physics, Shri Gavisiddeshwara Arts Science and Commerce College, Koppal, India**
[*]*manjuna999@gmail.com*

Room-temperature Zero Field NMR (ZFNMR) signals of bulk cobalt and Carbon Encapsulated Cobalt Nanopowder (CECN) were compared. Bulk cobalt exhibits two phases—FCC and HCP—producing two pairs of NMR signals, while CECN shows only a single FCC-related pair. Powder XRD confirmed the FCC phase in CECN. The results highlights the ability of $^{59}$Co IFNMR in identifying the phase composition of ferromagnetic materials.

**c0103**

**Impact of $BaZrO_3$ Nanostructures on the Functional Enhancement of $GdBa_2Cu_3O_{7-x}$ Coated Conductors for High-Field Superconducting applications**

Chandra Shekar Gantepogu[1,], Chia-Ming Yang[2], Peramaiyan Ganesan[1], In-Gann Chen[2], and Maw-Kuen Wu[1*]

[1]*Institute of Physics, Academia Sinica, Taipei, Taiwan*
[2] *National Cheng Kung University, Taiwan*
**Corresponding author:mkwu@phys.sinica.edu.tw*
This study systematically examines how introducing artificial defects affects the flux pinning mechanism and superconducting properties of $GdBa_2Cu_3O_{7-x}$ (Gd123) thin films. Specifically, the enhancement of the irreversibility field and flux pinning was achieved by incorporating $BaZrO_3$ (BZO) nanostructures into the Gd123 matrix. These films were deposited on ion-beam-assisted-deposition (IBAD) MgO substrates buffered with $(La,Sr)MnO_3$. The formation of a self-assembled BZO nanostructure network within the superconducting matrix significantly enhanced vortex pinning energy and the irreversibility field (Hirr) under magnetic fields applied along the c-axis. As a result, these coated conductors exhibit superior in-field performance compared to previously reported Gd123 systems, demonstrating the effectiveness of BZO nanostructure engineering for high-field applications.

**c0104**

**Structural and Magnetic Properties of Cobalt Ferrite Nanoparticles for Photocatalytic Dye Degradation Application**

Rahul Pandit1,a), Pranjali J. Aute2, Sagar Bhagde1, Sudarshan Gawali3, S. D. More1 and K. M. Jadhav3,4
*1Deogiri College, Chhatrapati Sambhajinagar (M.S.), India-431 005.*
*2CSMSS College of Polytechnic and Engineering, Chhatrapati Sambhajinagar (M.S.), India-431 011.*
*3Department of Physics, Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar (M.S.), India-431 004.*
*4Department of Physics, School of Basic and Applied Sciences, MGM University, Chhatrapati Sambhajinagar, (M.S.), India-431 003.*
** rahulpanditr75@gmail.com (Email of corresponding author)*

The structural and magnetic properties of cobalt ferrite nanoparticles synthesized via glycine assisted sol-gel auto-combustion synthesis are reported here. X-Ray diffraction tool was used to determine the phase purity, crystal structure and structural, infrared parameters. The crystallite size of the order of 23 nm was obtained from Scherrer equation. The lattice constant (8.3834 Å) well matches with the literature value. The XRD pattern show no extra reflections other than cubic spinel structure ensuring single phase formation. The vibrational studies were carried out by Fourier Transform Infrared Spectroscopy technique. The spectra reveals two absorption bands, one near 545 $cm^{-1}$ and other near to 393 $cm^{-1}$. The cobalt ferrite nanoparticles exhibit typical hysteresis curve showing saturation magnetization of the order of 78 emu/g. The enhanced magnetic values are due to the nanoparticle size

# d) Experimental techniques and devices

**d0001**

**Development of A Polycapillary Based Setup for Micro-XRF Elemental Mapping At BL-16 Beamline, Indus-2 Synchrotron Radiation Source**

Ayushi Trivedi[1,2,*], Ajay Khooha[1], Pardeep Kumar[1], A.K.Singh[1] , M. K.Tiwari[1,2]

*[1]Accelerator Physics and Synchrotrons Utilization Division, Raja Ramanna Centre for Advanced Technology, Indore, 452013, India.*

*[2]Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400094, India*

**Email:ayushit@rrcat.gov.in*

In the present work, we report design and development of a compact X-ray focusing setup based on polycapillary optics at the experimental station of the BL-16 beamline, Indus-2 synchrotron radiation source. The system consists of 5-axis (x,y, z, θ, φ) motions for the alignment of Polycapillary optics and 4-axis (x,y, z, φ) motorized motions for sample positioning. An X-ray CCD camera and knife edge scanner alongwith photodiode have been incorporated in the setup for precise alignment and accurate beam spot size determination of the focussed x-ray beam. At an incident energy of 12 keV, measured focussed x-ray beam size (vertical and horizontal directions) was found to be ~ 41 μm. This focussed x-ray beam was utilized for microXRF elemental mapping of a copper grid structure. We expect that this setup will significantly enhance the capabilities of the BL-16 beamline for combined micro-XRF and micro-XANES elemental mapping applications, especially for larger size samples.

**d0002**

**Fundamental Principles, Structural Design, And Advanced Applications Of Single-Electron Transistors**

Abhilasha Saini[1,*], Shubham Tiwari[1], Pinky Steffi[2], Sudhir B.[3]

*[1]Dept. of Engg., Sciences & Humanities, Thakur Shree DPS college of Engg.& Mgnt., Palghar, India*

*[2]Department of Humanities & Applied Sciences, Atharva College of Engg. Mumbai India*

*[3]Govt. College of Engineering & Technology, Bikaner, India.*

*[*]Email: abhilasha.saini@tsdcem.ac.in*

The basic ideas behind Single-Electron Transistors (SETs) are thoroughly examined in this article, with particular attention paid to the devices' design, workings, and the quantum mechanical processes that control their behaviour. The extensive range of implementations of SETs in various domains, namely the gas sensing technologies, logical circuitry, memory storage systems, and artificial neural networks, is methodically explored in this paper. The research also critically compares these implementations with foregoing reporting in these literary texts, foregrounding both execution approach upgradations and divergences. By delving into the advantages and implicit difficulties of these technologies, the paper focuses to clarify the prospects and impediments of SETs in recent and developing technological environments, placing recent advancements within a more comprehensive contextual analysis.

**d0003**

**Measurement of Diethorn Constants of Ar+$CH_4$ filled X-ray Proportional Counter**

Uday Singh[1], Shylaja Devan[2], Arkaprabha Bhowmik[2] and Shraddha S Desai[2,a)]

*[1]National Institute for Science and Educational Research, NISER, Jatni, Bhubaneshwar, Odisha, 752050*

*[2]Solid State Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400085*

**Email: ssdesai@barc.gov.in*

X-ray proportional counters for energy Spectroscopy are used for various applications such as X-ray fluorescence spectroscopy, thin film thickness gauging and Mossbauer studies. Gas filled proportional counters with high Z gases Ar or Kr show good detection efficiency for photons in soft X-ray region <50 keV, as well as Kr shows absorption edge at 14 keV. Linear range of gas gain is essential for accurate calibration of energy and thus any variation in X-ray energy due to absorption, emission, Mossbauer effect will be recorded accurately. Avalanche formation in proportional counters determine internal gas amplification factor i.e. gas gain. The linear region of Diethorn plot reflects proportional region accurately. Diethorn gas constants are measured for Ar+$CH_4$ (9:1) gas using the pulse mode operation. These values of Gas constants for the given purity level of the gas are derived with good accuracy. These values are very useful to determine the operation parameters of any detectors with complex anode-cathode geometry and filled with the given gas purity.

**d0004**

**Molybdenum Diselenide prepared at different times and temperatures as an electrode for hybrid capacitors**

*Shweta Tanwar[1*], Anurag Gaur[1], Nirbhay Singh[3], and A.L. Sharma[2]*

*[1]Department of Physics, Nataji Subhas University of Technology, New Delhi, India-110078*

*[2]Department of Physics, Central University of Punjab, Bathinda, India-151401*

*[3]Department of Applied Physics, School of Engineering and Technology, Amity University Gwalior, Madhya Pradesh- 474005, India*

**Email: sh1994t@yahoo.in*

In this article, we report the role of time and temperature during synthesis on the electrochemical behaviour of the prepared pure molybdenum diselenide via the hydrothermal route. The structural confirmation of MoSe2 was performed using X-ray diffraction and the Fourier transform infrared technique (FTIR). Here, the effect of preparing MoSe2 at different time durations and temperatures on the electrochemical behavior of the symmetric cell has been explored. The maximum specific capacitance was

observed for MoSe2 prepared at 180°C for 12 hours. Its value was detected to be around 251 F g-1 (at 100 mV s-1) with an energy density of 30 Wh kg-1 at 3 A g-1. Hence, the electrochemical results indicate that the MoSe2 material can be prepared at a low temperature and in a shorter time using the hydrothermal method, exhibiting high electrochemical performance, which makes it suitable for efficient energy storage devices.

**d0006**

**Synthesis, Characterization and Application of GdMnFe2O4 as an Advanced Humidity Sensor**

Bhavna Rohilla[1], Gyanendra Sheoran[2,*], Surender Duhan[1], Priya Malik[2] and Aryan Boora[1]
[1]*Advanced Sensors Lab, Department of Physics, Deenbandhu Chhotu Ram University of Science and Technology, Murthal, (Sonipat)-131039, Haryana, India*
[2]*Advanced Research in Optical and Microwave Applications (AROMA) Lab, Department of Applied Sciences, National Institute of Technology Delhi, Delhi, India*
**Email: gsheoran@nitdelhi.ac.in*

Gadolinium doped manganese ferrite ($GdMnFe_2O_4$) shows great potential for humidity sensing due to its improved electrical and adsorption properties. Doping with Gd enhances water vapor adsorption, leading to a notable change in resistance with varying humidity. Compared to undoped ferrite, $GdMnFe_2O_4$ exhibits better conductivity and faster response (7 s) and recovery (6 s) times, making it suitable for applications in environmental monitoring and industrial sensing.

**d0007**

**Fabrication and Characterization of Benzaldehyde Molecular Schottky Junction with Magnetic Electrode**

R Mallikarjun[1,2], Subramanya Hanumanu Sai[1], Rajeev Joshi[1,*]
[1]*Department of Physics, School of Physical Sciences, Central University of Karnataka, Kalaburagi, India-585367*
[2]*Department of Electronics and communication Engineering, Alliance college of Engineering and Design, Alliance University, Bengaluru, India-562106*
**E-mail: rajeevsj@cuk.ac.in*

In this study, we aim to understand the flow of spin in the junction between a metal and a semiconductor by attaching benzaldehyde molecules covalently onto silicon (100) surfaces. This attachment process is facilitated by thermal grafting, which involves the use of silicon-hydrogen (Si-H) groups on the surface. The goal is to create a catalytically active environment, particularly for the ferromagnetic nickel electrode. We investigate how the movement of spin current is influenced in the junction where a ferromagnetic nickel electrode meets a semiconductor (p-Si) by attaching benzaldehyde molecules to the silicon surface. By altering the arrangement of molecules at the junction, we observe changes in the total dipole moment. This change is significant because it affects the magnetoresistance (MR) (the change in electrical resistance under the influence of an external magnetic field) within the junction. We examine the electrical characteristics of the fabricated junction, Ni/C7H6O/p-Si/Al, by studying both the current-voltage relationship and the capacitance-voltage behavior. This helps us understand how the spin current is affected by the application of a magnetic field. To analyze the electrical properties of the silicon wafer's surface, we employ a modified version of the field emission theory. This theory allows us to effectively track changes in the surface properties of the wafer under the influence of external electrical fields.

**d0008**

**Development Of Electron Gun with Deflectors for Enhancement Of IR Signal Post Electron Beam Irradiation On Condensed Phase Matter**

Chandrasekhar Rao K[1, a)], Rutisha Kotian[2], Daly Davis[2] and K G Bhushan[1]
[1]*Technical Physics Division, Bhabha Atomic Research Centre, Mumbai 400085*
[2]*S K Somaiya College, Somaiya Vidyavihar University, Mumbai*
*a) Corresponding author: kcsrao@barc.gov.in*

In this paper, we describe the development and testing of a low energy electron gun with the X-Y deflectors along with its scanning software. The algorithm implements the tracking mode type of scanning. The electron gun is tested and mounted with an experimental set-up developed for studying low energy electron induced chemistry in the condensed phase. It is observed that intensities of IR signal post irradiation are enhanced by nearly 5 times in comparison with intensities using electron gun without deflectors.

**d0009**

**In situ spectroscopy investigations under sever plastic deformation at high pressures**

Nirmal Sharma[1, 2], Vaishnavi Sharma[1], K. K. Pandey[1, 2, a)], H. K. Poswal[1, 2]
[1]*High Pressure & Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Mumbai, India.*
[2]*Homi Bhabha National Instistute, Anushaktinagar, Mumbai, India.*
[a)] *Corresponding author: kkpandey@barc.gov.in*

An integrated confocal micro-Raman and ruby fluorescence imaging setup has been established for rotational diamond anvil cell based *in situ* investigations on materials subjected to severe plastic deformation at high pressures. With a spatial and depth resolution of ~ 2μm and 40μm, respectively, the setup can be used for Raman piezometry and stress components mapping across entire sample at sample-anvil contact surface. The ruby fluorescence imaging with 10x optical magnification can be used for

displacement field measurements in sample utilizing digital image correlation (DIC) method. A few benchmark experiments have been carried out to validate capabilities of the system.

**d0010**

**Energy Dependent X-ray Induced Modifications in Potassium Acid Phthalate Crystals: A Study at BL-03 Beamline, Indus-2 Synchrotron Radiation Source**

Shruti Gupta[1,2 *], Rajkumar Gupta[1], Praveen K.Yadav[1] Amit Saxena[3], Rajeev Bhatt[2, 3], Indranil Bhaumik[2, 3], and Mohammed H. Modi[1, 2]

[1]*Accelerator Physics and Synchrotrons Utilization Division, Raja Ramanna Centre for Advanced Technology, Indore 452013 INDIA.*

[2]*Homi Bhabha National Institute, Anushakti Nagar, Mumbai 400094, INDIA.*

[3]*High Energy Lasers and Optics Division, Raja Ramanna Centre for Advanced Technology, Indore 452013 INDIA.*

**Email:guptashruti@rrcat.gov.in*

Potassium acid phthalate (KAP) crystals are used in soft X-ray diffraction optics, particularly due to their strong reflectivity and suitability for low-energy X-ray monochromators. However, their structural integrity under prolonged exposure to synchrotron radiation, especially at energies near absorption edges, remains a subject of significant interest. This study investigates energy-dependent changes in the diffraction characteristics of a KAP crystal, mainly positions and broadening of Bragg peaks after the sequential exposures at the BL-03 beamline of Indus-2. The primary aim is to understand how exposure to different photon energies 500 eV, 600 eV, and 1000 eV affect the soft x-ray diffraction profiles of the KAP crystal. Notably, we observed a more pronounced peak shifts and shape distortions at 500 and 600 eV exposures, compared to that of 1000 eV.

**d0011**

**Non-Volatile and Digital Memristive Switching in Solution Synthesized Nanostructured $VO_2$ Thin Film-Based Metal-Insulator-Metal (MIM) Devices**

Pawan Kumar Ojha[1, a)], Dip Manna[1], Koushik Mondal[1], Supratic Chakraborty[1] and Shrawan Kumar Mishra[2]

[1]*Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Kolkata 700064, India*

[2]*School of Materials Science and Technology, Indian Institute of Technology (BHU), Varanasi 221005, India*

**Email: pawankr.ojha.rs.mst18@itbhu.ac.in*

In this study, we demonstrate the resistive switching of solution-based $VO_2$ thin film device under the influence of bias voltage. Fabrication and characterization of Ag/$VO_2$/$SiO_2$/Si metal-insulator-metal (MIM) devices is described here where $VO_2$ is synthesized using sol-gel technique. Further, x-ray diffraction studies indicate crystalline structure of $VO_2$ thin film with (011) and (022) monoclinic planes. XPS spectra of the $VO_2$ thin film shows presence of $V^{4+}$ and $V^{3+}$ states at room temperature. A two order of binary threshold switching is found when the voltage sweeps from 0 V $\rightarrow$ 15 V $\rightarrow$ −15 V $\rightarrow$ 0 V. A finite current in the *I-V* characteristics observed for the devices at zero voltage bias proves its non-volatile properties. The XPS data indicates that the threshold switching is probably originates from a mixed contribution of oxygen vacancy and Joule heating effect.

**d0012**

**Synthesis of CdSe Quantum dots and Their Application in $SnO_2$/CdSe based heterostructure Light Sensitive Low-voltage Photo-FET**

Chetna Gautam[1], Sandeep Dahiya[2], Nikita Kumari[1], Anupam Giri[3], Bhola N. Pal[2], and Anup K. Ghosh[1*]

[1]*Department of Physics, B. H.U., Varanasi-221005,*

[2]*School of Material Science, Indian Institute of Science, B. H. U., Varanasi-221005.*

[3]*Department of Chemistry, University of Allahabad, Prayagraj- 211002*

**Email:akghosh@bhu.ac.in*

The CdSe (Cadmium Selenide) quantum dots (QDs) have been prepared using a cost effective and less complex hydrothermal method. The as-prepared QDs were approximately 3.4 nm in size which was determined by X-ray diffraction and transmission electron microscopy. For the study of optical properties UV-vis and photoluminescence spectroscopy were used. Furthermore, these QDs were used as a photosensitive semiconducting layer for the photo-field effect transistor (photo-FET) with $LiAl_2O_3$ as a dielectric layer and $SnO_2$ as an electron transport layer (ETL) for the sensing of UV and visible light. The fabricated photo-FET of CdSe QDs has shown the saturation mobility ($\mu_{sat}$), on/off ratio and, subthreshold swing (SS) of 7.251 $cm^2$/V-sec, $10^5$ and, 400 mV/decade under dark conditions. The $SnO_2$ thin film-based FET did not show any sensing for visible light and very less sensing for UV light, besides, $SnO_2$/CdSe QDs based photo-FET gives an increment in the saturation mobility and on/off ratio compared to its SnO2 based counterpart. This result is due to broad absorption of CdSe QDs which made it possible for sensing of wide range of light from UV to visible.

**d0013**

**Fabrication of Solution-processed CdS Quantum Dots/$SnO_2$ heterojunction UV-Vis Sensitive Low-Voltage Phototransistors**

Nikita Kumari[1], Sandeep Dahiya[2], Chetna Gautam[1], Bhola Nath Pal[2], and Anup K. Ghosh[1, a)]

[1]*Department of Physics, Institute of Science, BHU, Varanasi-221005, India.*

[2]*School of Materials Science and Technology, IIT BHU, Varanasi-221005, India.*

**Email: akghosh@bhu.ac.in,*

CdS Quantum dots (QDs) are promising material for visible light detection due to their direct band gap, (2.4 eV), processability, good photoconductivity, low cost, and good chemical/thermal stability. In this work CdS QDs were synthesized via hydrothermal method and characterized by XRD, TEM and UV measurement. Here a solution processed UV-Vis sensitive low voltage phototransistor based on bilayer heterojunction CdS QDs (as a photoactive layer) and $SnO_2$ (as a semiconducting channel layer) has been fabricated. The photogenerated electrons are readily transferred from the CdS (UV-Vis sensitive) layer to the $SnO_2$ (carrier transport) layer. Here, ion-conducting Li-$Al_2O_3$ thin film has been used as a gate dielectric. The fabricated heterojunction CdS QDs/$SnO_2$ based phototransistor shows excellent electrical properties, such as saturation mobility of 1.68 cm $V^{-1}$ $s^{-1}$ and on/off current ratio of $1.6 \times 10^5$ as compared to the single $SnO_2$ counterpart. These results demonstrate that the solution-processed CdS QDs/$SnO_2$ heterojunction phototransistor provides a better approach for improving the performance of UV-Vis phototransistors with low-cost and large-area processing.

**d0014**

**Influence of Top Electrode Material on Resistive Switching Behavior of $TiO_2$-based Random Resistive Switching Memory (RRAM) Devices**

Avijit Tudu and A. Rajanikanth*
*School of Physics, University of Hyderabad, Gachibowli, Hyderabad – 500046, Telangana, India.*
**Email: ammanabrolu@uohyd.ac.in)*

This work explores the impact of the Top Electrode (TE) material on the resistive switching (RS) behavior of nanostructured titanium dioxide ($TiO_2$) based RRAM devices. Top Electrodes Au and Cr has been studied for RRAM devices. The TE not only provides an electrical contact, but actively participates in the formation and dissolution of conductive filaments (CFs) and can influence the switching mechanisms. The SET and RESET voltage were studied for Au/$TiO_2$/FTO, and Cr/$TiO_2$/FTO devices. For the Au/$TiO_2$/FTO device the SET voltage was found in the positive region, while that for the Cr/$TiO_2$/FTO device it was found in the negative region. The devices retention and endurance properties were also studied. The resistive switching characteristics of $TiO_2$-based Random Resistive Switching Memory (RRAM) devices are significantly impacted by the oxidation reaction at the interface between the metal TE and the $TiO_2$ nanostructures.

**d0015**

**Synthesis and Optical Characterization of Lead Halide Perovskite Single Crystal $MAPbBr_3$**

Parthkumar Zadafiya[1]*, Pawan Kumar[1], Om Modi[1], Yogesh Sonvane[1]
*[1]Advanced Materials Lab, Department of Physics, Sardar Vallabhbhai National Institute of Technology, Surat 395007, India*
**Email: parthpatel97257@gmail.com*

This research focuses on the synthesis and optical characterization of lead halide perovskite single crystals: methylammonium lead bromide ($MAPbBr_3$) . Single crystal were grown using the inverse temperature crystallization (ITC) method, which leverages the unique temperature-dependent solubility of perovskite precursors in solvent like DMF. The $MAPbBr_3$ crystals were successfully synthesized and characterized using Photoluminescence (PL), Raman, and Fourier Transform Infrared (FTIR) spectroscopy to evaluate their optical and structural properties. The PL spectrum revealed a sharp emission at ~549 nm, confirming high crystallinity and low defect density. Raman analysis identified characteristic vibrational modes corresponding to Pb–Br bonds and $MA^+$ ions, indicating strong organic–inorganic coupling. FTIR results supported the structural integrity and purity of the synthesized material. The results demonstrate the effectiveness of ITC for growing high-quality perovskite single crystals and lay the groundwork for advanced optoelectronic applications.

**d0016**

**Study of host to activator energy transfer in $ZrO_2$: $Sm^{3+}$ phosphor through photoluminescence analysis**

Sandeep Kumar[1], Ishant Kumar[1], Avinash Kumar[1], Rajesh Kumar[1] and Arvind K Gathania[1, a]
*[1]Departement of Physics and Photonics Science, National Institute of Technology, Hamirpur*
**Email: akgathania@nith.ac.in*

This work explores the development and characterization of ZrO2 incorporated with Sm3+ ions at different doping levels, synthesized using a solution combustion technique. The phase properties of the produced phosphor materials were investigated using the XRD technique, which shows that monoclinic phase of ZrO2 predominates with a tiny peak of the tetragonal phase in doped samples. Pl spectra of ZrO2 recorded at 285 nm excitation shows strong emission in the range of 400 – 650 nm, while some additional emission bands due to transitions 4G5/2→6H5/2, 4G5/2→6H7/2 and 4G5/2→6H9/2 of Sm3+ ions, in doped samples. Beyond 0.3 mol% doping, a concentration quenching effect of Sm3+ ions was seen. PL data of the samples further utilized to study the energy transfer from ZrO2 to Sm3+ ions.

**d0017**

**Synthesis of LiF/CsI:Tl Composite And Scintillation Characterization**

H. Kumawat[1,2], A.Tipnis[1,3], S.G. Singh[1,2], G.D. Patra[1,2], Shashwati Sen[1,2,a)]
*[1]Technical Physics Division, Bhabha Atomic Research Centre, Mumbai*
*[2]Homi Bhabha National Institute, Mumbai*
*[3]Indian Institute of Technology Patna, Bihar*

*Email: shash@barc.gov.in
A polycrystalline LiF/CsI:Tl composite is developed and characterized to check the feasibility of thermal neutron detection. CsI:Tl, an efficient scintillator with PSD ability, is combined with LiF containing natural occurring 6Li isotope that have high absorption cross section for thermal neutrons. The LiF/CsI mix was homogenized via ball milling and dehydrated under vacuum to remove residual moisture. The composite was uniaxial cold-pressed to make it compact and introduce translucency for better light collection. The scintillation properties were measured and alpha sensitivity observed in the LiF/CsI:Tl. The figure of merit (FOM) for discriminating alpha and gamma is approximately 2.

**d0018**

**Lead-Free $Cs_2AgBiBr_6$-Based Self-Biased Photodetector via One-Step Vapor Deposition**

Iman Biswas[1, *] and Aniruddha Mondal[1]
[1]*Department of Physics, National Institute of Technology Durgapur, Durgapur 713209, India*
**Email: imanbiswas08@gmail.com*

We report the fabrication and characterization of a self-powered photodetector based on lead-free $Cs_2AgBiBr_6$ thin films synthesized via a one-step thermal vapor deposition method. The resulting films exhibit excellent phase purity, uniform grain morphology, and strong optical absorption. A vertical ITO/$Cs_2AgBiBr_6$/Ag device was constructed and evaluated under white-light illumination (0.5 mW/cm$^2$). The device demonstrates a low dark current, clear rectifying behavior, and a significant photocurrent enhancement at zero bias, confirming effective internal electric field-driven carrier separation. The detector showed a rise and decay time of 125/350 ms with an on/off ratio of ~70. The calculated responsivity and detectivity were found to be ~$3.3 \times 10^{-3}$ A/W and ~$3.2 \times 10^{10}$ Jones, respectively, under zero bias. These results establish vapor-deposited $Cs_2AgBiBr_6$ as a promising, stable, and environmentally benign material for low-power optoelectronic applications.

**d0019**

**Lead-Free $Cs_3Bi_2I_9$-Based Resistive Switching Memory Device for Artificial Synapse Emulation**

Subhasish Chanda[1*], Iman Biswas[1], Rajeev Gupta[2] and Aniruddha Mondal[1]
[1]*Department of Physics, National Institute of Technology Durgapur, Durgapur 713209, India.*
[2]*Department of Physics, School of Engineering, University of Petroleum and Energy Studies, Dehradun, 248007, Uttarakhand, India.*
**Email: subhasishchanda99@gmail.com*

Lead-free halide perovskite-based resistive switching memory devices (RSMDs) are promising for next-generation memory and neuromorphic systems due to their straightforward fabrication and non-toxic nature. In this study, we report a lead-free RSMD based on Cs3Bi2I9 thin films (TFs), fabricated via low-cost, solution-processed spin-coating method. The X-ray diffraction spectra revealed a phase-pure Cs3Bi2I9 with high crystallinity and an indirect bandgap of ~2.22 eV was estimated from the optical absorption spectra. The Al/Cs3Bi2I9/ITO device exhibits stable bipolar switching with good ON/OFF ratio (~10) and excellent endurance over 500 consecutive cycles. In addition to the memory functions, the device successfully emulates key synaptic behaviors under various electrical pulse stimulations. These results highlight the potential of Cs3Bi2I9 material in mimicking biological synapses, establishing it as a promising candidate for next-generation non-volatile memory and artificial synaptic devices.

**d0020**

**Hardness, Thermal and Structural Properties of Lithium Alumino-borosilicate Glasses**

Kajal Dadwal[1], Atul Khanna[1, a)]
[1]*Department of Physics, Guru Nanak Dev University, Amritsar-143005, Punjab, India*
**Email: atul.phy@gndu.ac.in*

Lithium alumino-borosilicate glasses of composition: 20Li2O3-20B2O3-xAl2O3-(60-x)SiO2 ( x= 5,7.5, 10 and 12.5 mol%) were prepared by melt quenching technique in a temperature range of 1500- 1600°C. Glass samples were characterised by differential scanning calorimetry. The B-O co-ordination environments were determined by 11B Magic angle spinning nuclear magnetic resonance (MAS-NMR) spectroscopy. The short-range structure of glasses consists of BO3 and BO4 units. Glass density was measured by Archimedes' method and the hardness of samples by Vickers indentation. It is found that the glass transition temperature (midpoint value) increases from 520 to 536°C as the Al2O3 content is increased, while the hardness decreases from 5.03±0.01 to 4.74±0.09 GPa.

**d0021**

**Characterization of neutron beam at DURGA facility, DHRUVA reactor by absolute measurement techniques**

Meghnath Sen[1, 3] *, Shamim Akhtar[1], Jayesthi Mali[1], Shobha Ghodke[1], Sudesh Tripathi[1], D. B. Kulkarni[1], P. K. Nayak[3], S. Mukhopadhyay[2, 3] and Sneha C[1]
[1]*Radiation Safety Systems Division, Bhabha Atomic Research Centre, Mumbai-400085, India*
[2]*Nuclear Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, India*
[3] *Homi Bhabha National Institute, Anushaktinagar, Mumbai-40094, India*
**Email: meghms@barc.gov.in*

The paper presents the absolute methodology for determination of neutron fluence rate at the irradiation position of DURGA facility, DHRUVA reactor (40 $MW_{th}$ power) using standard gold foil activation technique. An absolute standard, $4\pi\beta\gamma$ coincidence system along with a HPGe spectrometer was used for the determination of induced activity. Based on the cadmium difference method, the 'Cadmium Ratio' was found to be (9.62 ± 0.51). The thermal and epithermal neutron fluence rate were found to be $(1.18 \pm 0.02) \times 10^6$ and $(1.33 \pm 0.07) \times 10^4$ $n/cm^2/s$, respectively. The values will be extremely useful for the nationwide utilization of the facility for various nuclear and solid-state physics applications.

**d0023**

**Interaction of RhodamineB and DMF Studied by Spectroscopic Technique**

Amit Sharma
*Department of Applied Sciences, Bharati Vidyapeeth's College of Engineering, A4, Paschim Vihar, New Delhi-110023, India.*
**Email: draksharma5477@gmail.com*

The molecular structure, fluorescence and photo physics of Rhodamine dyes are affected by the chemical environment of the dyes. Therefore, it is significant to probe the chemical changes taking place between laser dyes and solvents. Fourier Transform Infrared spectrum of DMF is reported. Spectrum of RhodamineB in DMF is also reported. Shift in band position and change in intensity is observed when RhodamineB is added to DMF. These changes appear due to the interaction between DMF and RhodamineB.

**d0024**

**Micro-patterned Electroplated Indium on GaAs for X-ray Pixel Detector Integration**

Anuj[1,3], Harsh Tiwari[2,3], Ravi Kumar[3,5], Shailesh K. Khamari[3,5,*], Geetanjali Vashisht[3], Alexander Khakha[3], P. Maheshwari[4], V.K. Dixit[3,5] and T.K. Sharma[3,5]
*[1]National Institute of Technology, Surat, 395007, India,*
*[2]Institute for Excellence in Higher Education, Bhopal, 462042 India,*
*[3]Semiconductor Materials Lab, Semiconductor Lasers and Devices Division, RRCAT, Indore 452013, India*
*[4]Accelerator Controls & Beam Diagnostics Division, RRCAT, Indore 452013, India*
*[5]Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*
**Email: shaileshk@rrcat.gov.in(Email of corresponding author)*

We report the development of a technique for electroplating Indium micro-dot arrays on GaAs substrates, aimed at realizing X-ray pixel detectors. Using an optimized electroplating process and photolithography-defined patterns, uniform Indium dots of 300 µm diameter and 16 µm height are deposited with a 600 µm pitch. These are successfully bonded to a custom-designed printed circuit board (PCB) to enable simultaneous electrical readout of 80 pixels in a 4 × 20 matrix. The Indium layer shows good adhesion, reasonable roughness, and a controlled geometry, that is crucial for bonding. This work lays the foundation for fabricating GaAs-based pixel detectors for hard X-ray imaging applications.

**d0025**

**Managing non-stability in 2D non-layered PtS via ultra-thin oxide passivation for ultra-fast, broadband photodetection**

Rohit Dahiya and Mukesh Kumar*
*Functional and Renewable Energy Materials Laboratory, Department of Physics, Indian Institute of Technology Ropar, Rupnagar, Punjab – 140001, India*
**Email: mkumar@iitrpr.ac.in*

2D non-layered materials (2DNLMs) possess exceptional qualities like high mobility and higher active sites at surface than their layered counterparts. Their unsaturated dangling bonds lead to higher photoresponse but at the cost of prolonged carrier lifetime. Herein, we report on interfacing 2DNLM PtS with ultra-thin layer of wide-bandgap amorphous Ga2O3 to realize high-speed broadband photodetection. PtS-Ga2O3 based PDs show peak responsivity of 0.25 AW-1 at 300 nm of incident light, an increase of more than 120 times compared to bare PtS PD. In terms of speed, heterojunction-based devices show fast speeds of 277µs/258µs (rise/fall) as compared to 42 ms/46ms for bare PtS, reducing by more than 150 times and showing stability even after 7500 hours.

**d0026**

**Development of Algorithm for Measurement of DC and AC electrical properties for Cryogenic Setup**

Souradeep Mitra[1, 2] and Shovit Bhattacharya[2, 3,a)]
*[1] Reactor Control Division, Bhabha Atomic Research Centre*
*[2]Technical Physics Division, Bhabha Atomic Reearch Centre*
**Email: shovitb@barc.gov.in*

We have augmented a cryostat into a versatile, fully automated electrical properties measurement setup for operations between 300K and 1.5 K. The setup is housed within a 26 mm diameter stainless steel tube of length 2m. The sample holder on a copper block attached to the steel probe can accommodate various sample shapes and sizes, which can be contacted using solder able contacts. A SCADA based algorithm has been developed augment the cryostat to measure the AC and DC electrical properties of different samples. The algorithm also interfaces with the cryocooler to control and monitor different parameters of the sample. We have successfully applied this setup to measure electrical porperties of diverse materials on different types of substrates.

**d0027**

**Brain-Inspired Synaptic Learning with Side-Gated 2D $MoS_2$ Iontronic Memtransistors**

Puranjay Saha[1, a)] and Bikas C. Das[1]

*[1]Emerging Nanoelectronic Devices Research Laboratory (eNDR Lab), School of Physics, IISER Thiruvananthapuram, Trivandrum 695551, Kerala, India*

**Email: puranjay21@iisertvm.ac.in*

Memtransistors, which integrate the functionalities of both memristors and transistors, represent a significant advancement with promising applications in neuromorphic computing. In this study, we investigate the use of few-layer $MoS_2$ thin films, grown via chemical vapor deposition (CVD), to fabricate side-gated electrochemical memtransistor (memT) devices. The $MoS_2$ thin films were grown using a NaCl-assisted atmospheric pressure CVD technique at a low temperature of 700 °C. The devices exhibit a pronounced anticlockwise hysteresis in their transfer characteristics, indicative of non-volatile memory behavior, with an ON/OFF ratio of ~$10^2$.

**d0028**

**Development and Characterization of Fast-Response Hard X-ray detector based on SI-GaAs**

Harsh Tiwari[1,3], Anuj[2,3], Shailesh K. Khamari[3,5,*], Alexander Khakha[3], Ashish Agrawal[4,5], Y.S. Kashyap[4,5], Salahuddin Khan[3,5], V.K. Dixit[3,5] and T.K. Sharma[3,5]

*[1]Institute for Excellence in Higher Education, Bhopal, 462042 India,*

*[2]National Institute of Technology, Surat, 395007, India,*

*[3]Semiconductor Lasers and Devices Division, RRCAT, Indore 452013, India*

*[4]Technical Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400085, India,*

*[5]Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*

**Email: shaileshk@rrcat.gov.in*

A semi-insulating GaAs (SI-GaAs) detector is designed and fabricated for high-speed hard X-ray detection with nanosecond temporal resolution. The 350 µm thick detector shows a low leakage current of 8.5 nA/mm² at 300 K, responsivity of 0.15 A/W at 870 nm, and a temporal resolution of ~7 ns. The detector is tested in current mode at applied bias upto 100 V under synchrotron X-ray between 9 to 24 keV. The detector exhibits an increase in the signal magnitude with X-ray energy, which seems to be in reasonable agreement with theoretical calculations. These results highlight GaAs's superior absorption efficiency, fast carrier transport, and low noise, making it a strong candidate for fast and high-energy photon detection for advanced X-ray applications.

**d0030**

**MoSe2 Photodetector with Ultrafast Response and Enhanced Broadband Detection Capabilities**

Priya Rani [1, a)] and Mukesh Kumar [1, b)]

*[1]Functional and Renewable Energy Materials Laboratory, Department of Physics, Indian Institute of Technology Ropar, Rupnagar, Punjab – 140001, India*

**Email: priya.23phz0008@iitrpr.ac.in*

Transition metal dichalcogenide (TMDC) Molybdenum Diselenide MoSe2 has a tunable bandgap, high mobility, and high responsivity, among other features, making it a promising material for a broadband photodetector. However, challenges remain in achieving larger-area growth and low response times with high responsivity. Here, we fabricate a large area MoSe2 photodetector device using thermally assisted conversion (TAC), followed by gold interdigitated electrodes deposited via thermal evaporation. Raman spectroscopy confirms the high-quality growth. The photodetector exhibits a broad photo-response with a peak responsivity of 0.186 A/W at 900 nm under a 5V bias. In addition to its large area, the device shows an ultrafast response time of 15.8 µs for 532 nm light. These results highlight the potential of TAC-grown MoSe2 for next-generation, large-area, ultrafast broadband photodetectors.

**d0031**

**Exploring the Use of Piezoelectric Quartz Tuning Fork Transducers in Mid-IR Gas Sensing for $SF_6$ Gas**

Ravi Chaudhary[1, *], M Sadique[1], S Chavhan[1], J K Fuloria[1], R G Ochnai[1], A M Kasbekar[1], R. B. Ingole[1] and T K Saha[1]

*[1]Technical Physics Division, Physics Group, Bhabha Atomic Research Centre, Mumbai-400085*

**Email: rchaudhary@barc.gov.in*

We present the development of a compact and robust mid-infrared gas sensing system based on quartz-enhanced photoacoustic spectroscopy (QEPAS) employing a piezoelectric quartz tuning fork (QTF) transducer for the selective detection of sulfur hexafluoride ($SF_6$). The system utilizes a distributed feedback quantum cascade laser (QCL) operating at 10.6 µm, modulated for second harmonic (2f) wavelength modulation spectroscopy. A commercial ~32.7 kHz QTF with a custom acoustic detection module and micro-resonator tubes achieves efficient acoustic coupling. Under optimized low-pressure conditions (~225 Torr), the system achieved a minimum detection limit (MDL) of ~75 ppb with excellent signal-to-noise ratio. Compared with conventional microphone-based photoacoustic cells, the QTF-based approach offers higher immunity to environmental noise, compactness, and field-deployable capability. These results confirm the viability of MIR QEPAS for real-time, portable monitoring of greenhouse gases.

**d0032**

**Investigation Of The Optoelectronic Behaviour Of Erbium Sulfate Crystals**

M. Rafia[1, a)], F.A. Najar[2], G.B. Vakil[1]
[1]*Department of Physics, University of Kashmir, Srinagar 190006, India*
[2]*Department of Physics, GDC Sumbal, Bandipora 193501, India*
**Email: rafiamushtaq987@gmail.com*

Erbium Sulfate crystals were grown by slow evaporation solution growth technique and systematically characterized to investigate its structural and optoelectrical properties. The X-ray diffraction analysis shows that these crystals have a monoclinic crystal structure with C2/c space group. The information extracted from transmittance and reflectance spectra proved helpful in determining refractive index, extinction coefficient and various other parameters for these crystals. Parameters like band gap, nonlinear refractive index, optical electronegativity, were also evaluated for these crystals. These findings demonstrate the potential of Erbium Sulfate as a candidate for optoelectronic device applications.

**d0033**

**Thermal Driven Magnon Spin Currents in YIG Single Crystals and Detection**

K. K. Kumawat[1, 2,*], A. Jain[1, 2], and S. M. Yusuf[2, 3,]
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*
[3]*UM-DAE Centre for Excellence in Basic Sciences, Mumbai 400098, India.*
**Email: kishorkk@barc.gov.in*

We report investigation of thermally excited magnon spin current in a single-crystal yttrium iron garnet ($Y_3Fe_5O_{12}$, YIG) via longitudinal spin Seebeck effect (LSSE). This spin current is injected into an adjacent non-magnetic metal layer (Pt) and converted into a measurable charge voltage through inverse spin Hall effect (ISHE). The efficiency of spin-to-charge conversion and the overall thermoelectric performance can be enhanced by optimizing combination of the magnetic material and the metallic layer. Measurements were carried out using a custom-built LSSE experimental setup, enabling precise control of thermal gradients and magnetic fields. Furthermore, $V_{ISHE}$ increases linearly with the applied temperature gradient, reaching a maximum value of 2.1 μV at $\Delta T$ = 20 K under a magnetic field of 1.8 kOe. These results demonstrate the reliability of our LSSE measurement setup and confirm the potential for optimizing spin caloritronics performance through interface and material engineering.

Keywords: Spin Seebeck effect, Spin Current, Spintronics, Inverse spin Hall effect.

**d0034**

**Spinel $CuGa_2O_4$ based Memristor Enabling Bipolar Switching and Analog Tunability for Next Generation Memory Devices**

Ayan Chatterjee, Mahesh Kumar[2a]
[1] *Department of Physics, IIT Jodhpur, Jodhpur 342030, India*
[2] *Department of Electrical Engineering, IIT Jodhpur, Jodhpur 342030, India*
**Email: mkumar@iitj.ac.in*

As conventional memories face limits in scalability, volatility, and energy use, resistive RAM (RRAM) has emerged as a strong candidate for next-generation memory and neuromorphic computing. Complex oxides, with greater structural and compositional flexibility than binary oxides, enable finer control of switching behavior. Here, we investigate $CuGa_2O_4$, a complex spinel oxide, which shows stable bipolar switching at low voltages, high endurance, and strong retention—ideal for low-power memory. Switching is driven by $Ag^+$ ion migration and conductive filament formation/dissolution. Beyond memory, the device supports analog switching, highlighting its potential for multifunctional memory and neuromorphic applications.

**d0035**

**Intrinsic Analog Switching in $AgHfO_{3-x}$ Memristors via Lattice-Derived Ag Filaments for Stable Synaptic Function**

Swaraj Mukherjee[1], Mahesh Kumar[2a]
[1] *Department of Physics, IIT Jodhpur, Jodhpur 342030, India*
[2] *Department of Electrical Engineering, IIT Jodhpur, Jodhpur 342030, India*
**Email: mkumar@iitj.ac.in*

$HfO_2$-based memristors excel in CMOS compatibility but suffer from stochastic filament growth and poor analog tunability, which limits their applications in neuromorphic systems. Here, we introduce $AgHfO_{3-x}$, an intrinsic silver-perovskite memristor that forms hybrid Ag–vacancy filaments without external active electrodes. Controlled oxygen incorporation during sputtering stabilizes switching, yielding an improved ON/OFF ratio, endurance >500 cycles, and retention $>10^4$ s (Figure 1). The device demonstrates analog potentiation/depression, paired-pulse facilitation, spike-number/width-dependent plasticity, and Pavlovian conditioning, highlighting its potential as a hardware synapse.

**d0036**

**Compact electron spectrometer for characterization of fast electrons spectrum generated in pulsed laser-matter interaction**

K. C. Gupta[1, a], P. Leshma[1], H. K. Poswal[1], K. K. Pandey[1], Gaurav Singh[2], Raghwendra Kumar[2], A. K. Poswal[3] and T. Sakuntala[1]

[1]*High pressure & Synchrotron Radiation Physics Division,* [2]*Technical Physics Division,* [3]*Atomic & molecular Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai*
**Email: kcgupta@barc.gov.in*
We have designed and developed a compact electron spectrometer to characterize the energy distribution of fast electrons generated from pulse-laser-matter interaction. The spectrometer is flange mountable with a provision for mounting permanent magnets without disturbing vacuum of experimental chamber. Energy-dispersed electrons from the dipole magnet are recorded at a lateral DRZ scintillating screen covered with 11µm thick Aluminum foil and coupled with a low noise CCD camera as a detection system. Measured (using hall probe) and simulated (using COMSOL software) spatial profiles of magnetic field in the electron propagation plane are found to be in close agreement. Electron energies at the screen were calibrated using simulated magnetic field and PIC code based PASUPAT software. The spectrometer has been installed and tested at a high power short pulse 200TW (5 Joule, 25fs, $I_{max}$~$10^{19}$ W/cm$^2$) Ti-Sapphire laser system with different thin metal foil targets.

**d0037**
**Structural and Elastic Analysis of DCH-32 Cotton Fiber using XRD data**
Manju V V[1*], Vinayakprasanna N Hegde[1], Divakara S[1], and Somashekar R[2]
[1]*Department of Physics, Vidyavardhaka college of Engineering, Mysuru-570002, India*
[2]*Center for Material science, University of Mysore, Vijnana Bhavan, Mysuru-570006, India,*
**Email: manjuvv@vvce.ac.in*
This study investigates the structural and elasto-mechanical properties of DCH-32 cotton fiber employing powder X-ray diffraction and a few computational analyses such as Match! and FullProf. Structural refinement Rietveld refinement confirmed a 100% match with the known crystal phase of cellulose. The refined data was further used to visualize the crystal structure and assess anisotropy. Elastic properties such as Young's modulus, shear modulus, linear compressibility, and Poisson's ratio were computed using ELATE. Results indicate mild anisotropy and stable mechanical behavior across crystallographic directions.

**d0038**
**Multicontrast X-ray Imaging with Crystal Analyser at Imaging Beamline of Indus-2**
Balwant Singh[1, 2,*)], Ashish K Agrawal[1, 2], Payal Singhai[1], Yogesh S Kashyap[1, 2], and Mayank Shukla[1, 2]
[1]*Technical Physics Division (TPD), Bhabha Atomic Research Centre, Trombay, Mumbai, India, 400085*
[2]*Homi Bhabha National Institute (HBNI), Anushaktinagar, Mumbai, 400094, India*
**Email: balwants@rrcat.gov.in*
We report development of a crystal analyzer based multicontrast X-ray imaging technique at Imaging beamline of Indus-2 synchrotron source. This technique employs a monochromatic X-ray beam and utilizes the rocking curve (RC) based angular selection/rejection property of a crystal analyzer to produce high sensitive multicontrast X-ray images of the specimen. This technique is capable of generating absorption/extinction, dark field/small angle scattering (SAXS) and differential phase /refraction contrast images of a sample, from a single set of experimental data acquired along various points of the RC curve. The multicontrast images offer complementary structural details of the specimens and complete utilization of the dynamic range. We discuss here comprehensive details of the experimental setup, working principle, data extraction and preliminary experiments to demonstrate merits of the developed setup.

**d0039**
**Elastic Behavior and Structure of Suvin Cotton Fiber using Powder X-Ray Diffraction**
Sofia Ranjini S[1*], Manju V V[2], Vinayakprasanna N Hegde[2], Hemaraju B C[3], B C Manjunath[1], and Somashekar R[4]
[1]*Department of Physics, Yuvarajas College, University of Mysore, Mysuru-570002, India*
[2]*Department of Physics, Vidyavardhaka college of Engineering, Mysuru-570002, India*
[3]*Department of Physics, Malnad College of Engineering, Hassan-573201, India*
[4]*Center for Material science, University of Mysore, Vijnana Bhavan, Mysuru-570006, India,*
**Email: kanirsofia@gmail.com*
This work explores the structural and elastic behavior of Suvin cotton fiber using powder X-ray diffraction and computational tools like Match! and FullProf. Rietveld refinement confirmed a complete phase match with cellulose, validating the structural model. The refined data was then used to visualize the crystal lattice and evaluate anisotropy. Using ELATE, key elastic parameters such as Young's modulus, shear modulus, linear compressibility, and Poisson's ratio were calculated. The results show low anisotropy and consistent mechanical stability along different crystallographic axes.

**d0040**
**Thermoresponsive Luminescence in $Mg_3WO_6:Tb^{3+}$ Double Perovskite Phosphor for Non-contact Optical Thermometry**
Naresh Degda[1, a)], Nimesh Patel[1], Rohan Arya[1], M. Srinivas[1]
[1]*Luminescence Materials Laboratory, Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara-390002, India*
**Email: degdanaresh65@gmail.com*

The thermoresponsive luminescence properties of $Mg_3WO_6:Tb^{3+}$ phosphor, synthesized via solid-state reaction, were investigated for contactless optical thermometry. The X-ray diffraction (XRD) of synthesized phosphor confirmed the monoclinic crystal structure of the material. Upon optical excitation (380 nm), the phosphor exhibits green photoluminescence (PL) emission at 490 nm and 550 nm, corresponds to $^5D_4$-$^7F_6$ and $^5D_4$-$^7F_5$ transitions of $Tb^{3+}$ ions, respectively. To examine the thermoresponsive luminescence of the material, the PL spectra of the phosphor were recorded at elevated temperatures within the range of 303-513 K. The temperature-dependent PL (TDPL) spectra shows that the $^5D_4$-$^7F_6$ and $^5D_4$-$^7F_5$ transitions demonstrating diverse responses to temperature, showing thermal dependence. Such energy states of phosphor are called thermally-coupled energy levels, contributing extensively optical thermometry. By using the fluorescence intensity ratio (FIR) from the TDPL spectra, the temperature sensing properties of the $Mg_3WO_6:Tb^{3+}$ phosphor was investigated. As a result, the maximum relative sensitivity $S_R$ was found to be 0.62% $K^{-1}$, attained at 303K. Additionally, the FIR values calculated for the heating and cooling processes, as well as the repeatability cycles, check the reliability and repeatability of the phosphor as a temperature sensor.

**d0041**

**Signature of proximity Induced Magnetic signature in Graphene/ Magnetic Insulator heterostructure**

Sandeep, Neesha Yadav, Nilesh Choudhury, Mayank Shukla, Pintu Das
*Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, 110016, India.*
**Email: pintu@physics.iitd.ac.in*

The recent discovery of magnetism in 2D materials stimulated the interest of the scientific community in the field of 2D magnets. While the most explored intrinsic ferromagnets such as CrI3, Fe3GeTe2 (FGT) and Cr2Ge2Te6, (CGT) etc. are unstable in ambient conditions, which presents a significant challenge. Therefore, there is a scope in exploring the externally induced magnetism in non- magnetic 2D materials via external perturbation, which can provide the stability in ambient conditions along with extra-ordinary electric properties. Theoretical study suggests robust Quantum Anomalous Hall effect in Gr/CGT heterostructure, due to small lattice mismatch & high SOC due to heavy Te atom at the interface. In this work, we demonstrated the proximity induced magnetism in the nano flakes of Graphene by fabricating a vertical stack of Graphene/CGT and performing low temperature magneto-transport measurements.

**d0042**

**Design of Multiwire Based Sense and Readout Electrodes for 2-Dimensional Position Sensitive Neutron Detector**

Shraddha S Desai*, Rohit Chandak, Vaibhav Kulkarni, Mala N Rao
*Solid State Physics Division Bhabha Atomic Research Centre, Mumbai*
**Email: ssdesai@barc.gov.in*

2-D position sensitive detector for neutron based on multiwire structure and delay line readout method is indigenously designed and is being fabricated. Position Sensitive Detector (PSD) gives the neutron intensity over the entire sensitive area unlike that of 1D PSD. Small Angle neutron scattering (SANS) Spectrometer at GT Lab consists of fan-like multiPSD system that gives neutron intensity distribution with near 2D sensitive area but with few blank spaces. Continuous data is essential for the thorough analysis of the sample. Multiwire grids are the heart of the 2D PSD and are responsible for determining the properties such as linearity and uniformity of the data. Uniform drift field and high electric field for avalanche formation depends on the microscopic perfection of these grids. Each grid consists of an array of equi-spaced wires and all these three grids are arranged in the gas volume. Design of grids, engraving the desired pattern and gold coating on the PCB of size 720 mm x 720 mm was a challenge. Gerber files for field grid, X and Y cathode grids and drift grids were generated. Readout grids have mounting pads for the L and C components for delay line, at the end of each wire. Details of the design and function of these grids is presented

**d0043**

**Evaluation of Third Order Nonlinear Optical Parameters of MXene by Z-scan Technique**

Kanisha Manwani, Jeevan Jyoti, Mamta Sharma and Surya Kant Tripathi*
*Department of Physics, Centre of Advanced Study in Physics, Panjab University, Chandigarh, 160014, India*
**Email: surya@pu.ac.in*

MXene ($Ti_3C_2T_x$) is synthesized through chemical etching technique from MAX phase precursor ($Ti_3AlC_2$) by removing "Al" using HF solution. The structure of MXene has been confirmed by X-Ray diffraction (XRD). The linear optical properties of $Ti_3C_2T_x$ MXene have been investigated by UV-Visible spectroscopy. The non-linear optical parameters such as non-linear refractive index ($n_2$), absorption co-efficient ($\beta$) & Third Order Susceptibility ($\chi^{(3)}$) have been calculated by using z-scan technique. The better value of Nonlinear Third Order susceptibility of MXene is due to Dielectric Confinement Effect.

**d0044**

**Enhancing $Cu_2O$/FTO Photodetector Performance and Spectral Selectivity through Carbon Dots**

Hosuru Satishkumar Reddy[1], Putha Kishore[1,*], D. Amaranatha Reddy[1] and M. Padmavathi[2]
[a] *Department of Sciences, Indian Institute of Information Technology Design and Manufacturing, Kurnool, AP, India-518007.*
[b] *Department of Physics, KVR GDCW Kurnool, Cluster University Kurnool, AP, India-518002.*
**Email: kishore.photonics@iiitk.ac.in*

In this study, carbon dots (CDs) were prepared using a microwave-assisted method, and a $Cu_2O$/FTO sample was fabricated using an electrochemical deposition method. Further, a CD/$Cu_2O$/FTO photodetector was prepared by incorporating the carbon dots by the drop casting method. The I-V characteristics of $Cu_2O$/FTO and CD/$Cu_2O$/FTO samples have been studied, and it was found that Cd/Cu2O/FTO shows better responsivity with 0.039 A/W and a Detectivity of $0.5 \times 10^{10}$ Jones at 632 nm. This work explores the addition of carbon dots to $Cu_2O$/FTO photodetectors, which facilitates charge separation and extended light absorption, resulting in the improvement of the spectral selectivity of visible light photodetectors.

**d0045**

**Analysis of Temperature induced effects on mid-infrared spectra of Astro mixtures**

Aayushi Raval, Debjani Bagchi
*The Maharaja Sayajirao University of Baroda, Sayajigunj, Vadodara, Gujarat, 390020, India*

The detection and analysis of astromolecules is not trivial. Various factors like conditions of Interstellar medium (ISM), molecular properties, observational techniques and instrumentation etc. can affect the detection and analysis of molecules present in space. The several conditions of ISM include density and temperature, radiation field, presence of dust grains and turbulence. In the present study, we have explored the temperature induced changes in the infrared spectra of pure molecules and mixtures. Isolation of prominent modes has been done and quantification of changes using relative intensity estimates. The machine learning analysis has been done with the help of clustering, principal component analysis and Nonnegative matrix factorization. Testing of machine learning algorithms has been carried out for higher accuracy. Different spectral demixing techniques have been tried out.

**d0046**

**Utility of chemiresistive hydrogen sulfide sensors for assessment of water quality**

Kailasa Ganapathi S[1], Ankita Pathak[1], Niyanta Datta[1], Rabi Datta, T. K. Saha, Manmeet Kaur[1, a)], N Rao A V S S[2],
[1]*Technical Physics Division, Bhabha Atomic Research Centre, Mumbai*
[2]*Advanced Genomics Section, BARC, Mumbai.*
**Email: manmeet@barc.gov.in*

Water is one of the most essential natural resources, and the sustenance of safe supply of water intended for human consumption is a worldwide challenge. Various physical, chemical, and biological parameters affect the water quality. One of the important aspects to be considered for water intended for human consumption is its potential toxicity associated with the microbial risks elicited by the presence of bacteria (often arising from human and animal feces). Guidelines for Drinking-Water Quality by world health organization (WHO) and other authorities support the use of bacterial indicators as a basis for assessing drinking water quality. So, depending on presence of total coliform organisms present per 100 ml of water, it has been categorized into three different classes with respect to its usage. In addition to various testing methods, testing for H2S release has been an accepted method for evaluation of water quality and is routinely being used across the world. In the present work, we have demonstrated the utility of indigenously developed chemiresistive H2S gas sensor to test the H2S released from water samples containing contaminating bacteria. This method is operator friendly, fast, economical and capable of evaluating the microbial quality of water within 10 h.

**d0047**

**A Digital Radial Shearing Interferometer for Stress Analysis: Design and Validation Using a Metallic Plate**

Sanjiva Kumar[1*], R. P. Shukla[2], S. Jena[1] and D. V. Udupa[1]
[1]*Atomic & Molecular Physics Division, Bhabha Atomic Research Centre, Mumbai 400 085*
[2]*Spectroscopy Division (Ret.), Bhabha Atomic Research Centre, Mumbai 400 085*
*****Email: *sanjivk@barc.gov.in*

The technique to perform non-contact analysis of stress in materials across various scales is crucial for ensuring their structural integrity and performance. This paper presents the design of a novel digital shearing interferometer developed for this purpose. The proposed shear device is an assembly of two telescopic lenses with 100 mm and 90 mm radii of curvature, one centrally fixed into the other, generating a radial shear of 1.21. The shearing interferometric technique has been demonstrated for stress analysis in a diffusing metallic plate mounted vertically on its lower edge.

**d0048**

**Development of $SnO_2$:CuO-Based Chemiresistive Hydrogen Sulphide Gas Sensor Using hybrid PVD Approach**

Damu V. Rupnar[1,2], Deepak Goyal[1], P. Sarawade[2], Niranjan S. Ramgir[1]
[1]*Gas Sensing Devices Section, Technical Physics Division, Bhabha Atomic Research Center, Mumbai 400 085*
[2]*Department of Physics, University of Mumbai, Kalina, Mumbai, 400 098*
**Email: niranjanpr@yahoo.com*

This study reports the development of a high-performance chemiresistive hydrogen sulphide ($H_2S$) gas sensor using a hybrid physical vapor deposition (PVD) technique. The sensor fabrication integrates two complementary PVD methods: Direct Current (DC) sputtering for tin (Sn) deposition and thermal evaporation for copper (Cu), forming a heterostructured $SnO_2$:CuO sensing layer. This approach significantly enhances gas adsorption and charge transfer properties. The resulting sensor exhibited a sensor response (SR) of 22,000 (Ra/Rg) towards 500 ppm $H_2S$, with rapid response and recovery times of 60 seconds and 300 seconds, respectively. The sensor's performance was evaluated against the 4-S sensor selection criteria Sensitivity, Selectivity, Stability, and

Suitability to assess its commercial viability. Consistent response kinetics observed over multiple cycles, including repeated high-concentration $H_2S$ exposures (500 ppm), confirm the excellent repeatability and reproducibility of the sensor. Long-term stability tests conducted over six months demonstrated that the sensor maintained an SR of 2,200 towards 10 ppm $H_2S$, with negligible degradation. Selectivity studies showed a significantly higher response to $H_2S$ compared to common interfering gases such as methane ($CH_4$), chlorine ($Cl_2$), ammonia ($NH_3$), and ethylene ($C_2H_4$). The synergistic combination of Sn and Cu, achieved through dual PVD deposition, enhances the sensor's sensitivity, selectivity, and durability. Meeting the 4-S criteria positions this sensor as a promising candidate for industrial and environmental $H_2S$ monitoring applications.

**d0049**

**Are Scanning Range Limits and Thermal Effects Skewing Your Z-Scan?**

Varun Tripathi[1], Sruthil Lal S.B[1], Soubhik De[1] and Alok Sharan[1,*]

*[1]Department of Physics, Pondicherry University, Puducherry, India - 605014*

**Email: aloksharan@pondiuni.ac.in.*

Z-scan technique is widely used for a quick estimate of the sign and magnitude of the third order optical nonlinearities in diverse materials. However, even under seemingly valid experimental conditions, accurate calibration of the setup, particularly the choice of focusing lens and technique of recording the transmitted intensity, remains non-trivial. These factors critically influence the accuracy and reliability of the extracted nonlinear parameters. In this report we demonstrate how insufficient scan range and the presence of long-lived thermal can impact accurate determination of nonlinear optical coefficients, specifically in liquid samples. We outline practical strategies to ensure accurate and reproducible measurements.

# e) Surfaces, interfaces and thin films

**e0001**

**Deep-UV Surface-Enhanced Resonance Raman Scattering Via GLAD-Fabricated Aluminum Nanorod Arrays**

Lakshay Bhardwaj, C. M. Vidhya, Shivam Singh, and J.P. Singh
*Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, 110016, India.*
**Email: lakshaybhardwaj12@gmail.com*

Surface-enhanced Raman scattering (SERS) enhances weak Raman signals via localized surface plasmon resonance (LSPR) in metallic nanostructures. Conventional silver and gold-based SERS substrates work efficiently under visible or near-infrared (NIR) excitation but show limited performance in the deep ultraviolet (DUV) region. Aluminum (Al), with its broadband plasmonic response extending from DUV to NIR, presents a viable alternative for UV-active SERS applications. In this study, we reported the fabrication of highly ordered and anisotropic Al nanorod arrays using the glancing angle deposition (GLAD) technique. GLAD offers precise control over nanorod orientation, spacing, and morphology, key parameters for optimizing plasmonic hotspots. The nanorods were deposited on glass substrates via electron beam evaporation and evaluated using a 266 nm excitation source. The fabricated arrays enabled sensitive and reproducible detection of adenine at a concentration of 0.1 mM, with strong signal-to-noise ratios and minimal background interference. This work demonstrates the potential of GLAD-engineered Al nanorod arrays as efficient, scalable, and cost-effective substrates for DUV-SERS-based molecular detection.

**e0002**

**Powder XRD and SEM Study of Mg-Doped MnS Metastable Thin Film Composites**

Poojashree[1,a)] and E Deepak D'Silva[2]
*[1]Department of Physics, St Philomena College (Autonomous), Puttur, Karnataka, 574202*
*[2]Department of Post graduate Studies and Research in Physics, St Aloysius (Deemed to be University), Mangaluru 575003, Karnataka, India*
*a) Email: poojavrai23@gmail.com*

Undoped and magnesium-doped MnS thin films (with 1, 3, 5, and 10 wt% Mg) were synthesized on glass substrates using the spray pyrolysis technique. Structural, optical properties of the films were studied. Powder X-ray diffraction (XRD) analysis revealed that the undoped MnS and Mg-doped MnS thin films (1%, 3%, and 5% Mg) exhibited an amorphous cubic zinc-blende structure (β-MnS). However, when the Mg doping concentration increased to 10%, the XRD pattern showed improved crystallinity, with the emergence of peaks corresponding to the hexagonal wurtzite structure (γ-MnS). The composition of thin film material was analyzed using EDS technique and found the formation of thin film composite. The thickness and the morphology of the thin film composite were measured using the SEM technique.

**e0003**

**A Study on Structural Properties of Zn-Doped CdO Thin Films**

Akash Arjun Bag[1),a)], E. Deepak D'Silva[1]
*[1]Center of Post Graduate Studies and Research in Physics, St Aloysius (Deemed to be University), Mangaluru, Karnataka 575003, India.*
*a)Email: akashbag7468@gmail.com*

Thin films of pure and zinc-doped cadmium oxide (CdO) were fabricated utilizing the spray pyrolysis method on glass substrates. An extensive analysis was conducted encompassing structural, morphological and compositional aspects of these films. Powdered X-ray diffraction (XRD) analysis unveiled that the deposited thin films possessed face-centered cubic structures characteristic of monteponite CdO. Field emission scanning electron microscope (SEM) images depicted distinct crystalline morphologies among the nanoscale thin films, varying with the dopant concentration. Energy-dispersive X-ray spectroscopy (EDS) spectra confirmed the presence of Cd, Zn and O in the samples.

**e0004**

**Characterization of Degenerate Zn-doped CdO thin films**

P. Sreenanda[1,a)], Divya[1], S. Trupthi[1], Akash Arjun Bag[1], E. Deepak DSilva[1]
*Department of Physics, St Aloysius (Deemed to be University), Mangaluru, Karnataka 575003, India.*
*a) sreenanda257@gmail.com*

Spray pyrolysis method was used to deposit pure and Zn-Doped CdO thin films on a glass substrate. A broad analysis was conducted of its optical and electrical properties. The optical absorption spectra showed a progressive increase in absorbance with rising $Zn^{2+}$ doping levels. Additionally, the optical band gap widened with Zn incorporation, reaching 2.71 eV for 1 wt% Zn, in contrast to 2.58 eV for undoped CdO. Both the refractive index and photoconductivity were found to be significantly influenced by the doping concentration. Electrical properties, assessed using Van der Pauw Hall effect measurements, demonstrated a clear decrease in electrical resistivity with increasing Zn content. As a result, the films exhibited favorable degenerate semiconductor characteristics. Photoluminescence (PL) spectra revealed enhanced visible emissions at 470, 575, and 630 nm due to $Zn^{2+}$ doping, which is attributed to the filling of $Cd^{2+}$ vacancies by $Zn^{2+}$ ions, indicating changes in defect density.

**e0005**

**Percolation threshold of Fe / CoFeB films on MgO: A comparative study using in situ resistance variation**

Vishal Tyagi[1], Dileep Kumar[2], Kavita Sharma[3], Gagan Sharma[1,*], Shubham Kumar[3] and V. R. Reddy[2]

[1]*Department of Physics, Faculty of Science, University of Allahabad, Prayagraj-211002, India*
[2]*UGC-DAE Consortium for Scientific Research, Khandwa Road, Indore-452001, India*
[3]*Center for Spintronic Materials, Amity Institute of Applied Sciences, Amity University, Noida-201313, India*
**Email: gagansharma@allduniv.ac.in*
In the present work, Fe and CoFeB films are examined in situ for investigating the percolation threshold of both the magnetic films on MgO. Thus resistance variation approach was followed in situ while depositing Fe and CoFeB films on the deposited MgO film. The structural quality and thickness of deposited magnetic film was ensured using X-ray reflectivity. The variation of resistance and rate of change of resistance with depositing film thickness indicates the Volmer-Weber growth for both the films. However, percolation threshold is observed to be higher for CoFeB film as compared to Fe which is due to low wettability of CoFeB on MgO. The results are important and directional in view of modification of growth process on MgO, which may further improve the interface dominating phenomena.

**e0006**

**The Role of Substrate Orientation On Uniform Growth Of $TiO_2$ Nanorods**

Kuri Manjunatha[1], Devarajan Alagarasan[2], R. Ganesan[3] and M. Ramudu[1, a)]
[1]*School of Sciences (Physics), National Institute of Technology Andhra Pradesh, Tadepalligudem – 534101*
[2]*Department of physics, Nitte Meenakshi Institute of Technology, Bangalore – 560064*
[3]*Department of Physics, Indian Institute of Science, Bangalore - 560012*
*a) Email: ramudu@nitandhra.ac.in*
A highly ordered, vertically oriented $TiO_2$ nanorods array is successfully synthesized on a fluorine doped tin oxide (FTO) conducting substrate with a facile and cost-effective synthesis using hydrothermal method. The effect of different preparation conditions on the growth morphology of $TiO_2$ nanorods was investigated. Field emission scanning electron microscopy results demonstrate large scale nanorods grown on the FTO substrate. The nanorods are well aligned at growth condition of FTO conducting surface facing downwards and kept at an angle of 45° for 60 min growth time. From cross sectional image of $TiO_2$ nanorods, we have analyzed the length of the nanorods and is found to an average of 1.6 µm. The X-ray diffraction results reveals that only the rutile phase is present. These results indicates that well oriented and single phase $TiO_2$ nanorods have been successfully grown.

**e0008**

**Study Of Thickness Variation With Deposition Time For Sputtering Grown Zinc Ferrite Thin Films**

Neha[1], Weon Cheol Lim[2], Sandeep Kumar[1], Keun Hwa Chae[2], and Jitendra Pal Singh[1, *]
[1]*Department of Sciences (Physics), Manav Rachna University, Faridabad, Haryana, 121010, India*
[2]*Advanced Analysis and Data Centre, Korea Institute of Science and Technology (KIST), Seoul 02792, South Korea*
**Corresponding author: jpsingh@mru.edu.in*
This research aims to determine how deposition time affects the thickness of zinc ferrite (ZF) thin films using Rutherford Universal Manipulation Program (RUMP) simulations of Rutherford Backscattering Spectroscopy (RBS) data. In this work, ZF thin films were synthesized using radio frequency (RF) sputtering under controlled conditions, with deposition times ranging from 2 to 105 min. The as-deposited thin films were annealed at 600 and 800 °C. RUMP simulations offer quantitative insights into film thickness and stoichiometry, confirming the presence of Zn, Fe, and O. As deposition time increases from 2 to 105 min, the thickness of the ZF thin film increases from 7 to 145 nm at both annealing temperatures. Thus, the thin film thickness increases with longer deposition times, as extended durations allow more atoms to accumulate on the substrate, leading to thicker films.

**e0009**

**Studies on Development of Composite Material as A Potential Substrate for Neutron Generator Target**

B. C. Nailwal[1,2, a], N Goswami[2], S. Vala[1,3], R. K. Lenka[1,4], Soumitra Kar[1,2], Rajesh Kumar[1,3], Tuhin Misra[2], K. T. Shenoy[5,]
[1]*Homi Bhabha National Institute, Mumbai, Maharashtra, 400094, India*
[2]*Alkali Material and Metal Division, Bhabha Atomic Research Centre, Mumbai, Maharashtra, 400085, India*
[3]*Institute for Plasma Research, Gandhinagar, 382428, India*
[4]*Powder Metallurgy Division, Bhabha Atomic Research Centre, Vashi, Navi Mumbai, Maharashtra, 400703, India*
[5]*Chemical Engineering Group, Bhabha Atomic Research Centre, Mumbai, Maharashtra, 400085, India*
[a]*Email: bipin@barc.gov.in*
A major issue with currently available targets of neutron generators is the delamination of hydrogen isotope-containing coatings during fabrication and testing. One of the primary causes of this delamination is the mismatch in thermal expansion between the coating material (Ti) and the substrate material (oxygen-free high-conductivity copper, OFHC Cu). In order to address this issue, the development of a composite material with high thermal conductivity and low thermal expansion has been undertaken. In this study, composites were developed using the powder metallurgy route, followed by sintering in a hydrogen atmosphere. The samples were characterized for their morphology and thermal conductivity. The composition containing 90 mol% Cu and 10 mol% W was found to be a promising candidate for use in neutron-based scanning targets.

**e0010**

**Crystallographic Reorientation and Grain Boundary Passivation in Ni–N Co-doped $CuCrO_2$ Thin Films for Enhanced Electrical and NIR Optical Properties**

JamshinaSanam P.K[1*],Midhun Shah[1, 2], P.P.Pradyumnan[1]
[1] *Department of Physics, University of Calicut, Malappuram, Kerala*
[2] *Department of Physics, Farook College, Kozhikode, Kerala,*
**Email:jamshinasanampk@uoc.ac.in*

This study investigates the distinct roles of nitrogen annealing and nitrogen co-doping in tuning the structural and electrical properties of Ni-doped $CuCrO_2$ (CCNO) thin films. Nitrogen annealing induced grain boundary passivation, reducing the potential barrier from 10.5 meV to 1.23 meV and improving mobility to 11.12 $cm^2 V^{-1} s^{-1}$. In contrast, nitrogen doping enhanced carrier concentration and electrical conductivity, achieving a peak value of 9159 S/m. Structural analysis revealed crystallographic reorientation due to altered adatom kinetics and surface energy modulation. NIR transmittance reached 84.4% at 2000 nm, while a Burstein–Moss shift indicated increased carrier density. Each process step—sputtering, nitrogen annealing, and doping—played a synergistic role in optimizing film performance. These results highlight the importance of process–dopant interactions in tailoring multifunctional $CuCrO_2$ thin films.

**e0011**

**Fabrication of Nanopatterned Flexible AuNPs@Grating@PDMS film for SERS Applications**

Kirti Singh[1], Rakesh S. Moirangthem[2] and P. M. Sarun[1]
[1]*Functional Ceramics Lab, Department of Physics, Indian Institute of Technology (ISM), Dhanbad 826004, India.*
[2]*Nanophotonics Lab, Department of Physics, Manipur University, Canchipur, Manipur, India – 795003.*
**Email:sarun@iitism.ac.in*

This study presents the fabrication and comparative analysis of flexible polymeric film-based surface-enhanced Raman spectroscopy (SERS) substrates, including pristine PDMS, AuNPs-embedded PDMS (AuNPs@PDMS), and AuNPs-embedded patterned PDMS (AuNPs@grating@PDMS). These substrates were fabricated using a simple curing process. AuNPs@grating@PDMS exhibited the highest SERS enhancement, attributed to the combined effects of periodic nanostructures and plasmonic hotspots from the embedded AuNPs. AuNPs@PDMS showed moderate enhancement due to the presence of AuNPs, while pristine PDMS showed minimal signal, as expected. These findings highlight the critical role of surface nanostructuring and nanoparticle accessibility in achieving strong SERS enhancement. The approach demonstrates a low-cost, flexible, and scalable route to fabricate effective SERS substrates.

**e0012**

**Investigation of Thermally Induced Changes in the Surface Microstructure and Nanomechanical Properties of NiTi Films**

Swapan Jana[1, a)], S.C Mishra[2], A.K Debnath[3], V.B Jayakrishnan[1], D. Bhattacharya[1, 4], and Surendra Singh[1, 4]
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India*
[2]*Materials Processing and Corrosion Engineering Division, BARC, Mumbai 400085, India*
[3]*Technical Physics Division, Bhabha Atomic Research Centre, Mumbai 400085 India*
[4]*Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*
[*] swapanj@barc.gov.in

Ni-rich NiTi films were deposited on Si substrates by RF and DC magnetron sputtering using Ni and Ti targets at a substrate temperature of 400 °C. Post-deposition annealing was performed at 600 °C in vacuum and Ar environments to investigate the effects of annealing conditions on the microstructure and nanomechanical properties. The films deposited at 400 °C were amorphous or partially crystalline, while annealing induced crystallization, confirming the presence of the martensitic B19' phase ($2\theta = 44.62°$) and Ni precipitation ($2\theta = 52.06°$). Films annealed in Ar exhibited enhanced crystallinity and larger grain size compared to those annealed in vacuum. The as-dep. film showed the maximum hardness (~5.07 GPa), which decreased to ~1.94 GPa after Ar annealing. The results also indicated the formation of a self-protective Ni and Ti oxide surface layer on the NiTi films, which could impart unique properties such as enhanced corrosion resistance, improved biocompatibility, and potential for application in microelectromechanical systems.

**e0013**

**Polarization dependence study of plasmonic nanoantenna substrates for Efficient Surface-Enhanced Raman Scattering**

Lekshmi J[1, a)], Shweta Deshmukh[1, b)] and Padmnabh Rai[1, c)]
[1]*School of Physical Sciences, UM-DAE Centre for Excellence in Basic Sciences, University of Mumbai, Mumbai-400098, India*
[a)] *Corresponding author: lekshmi.j@cbs.ac.in*

Surface-enhanced Raman spectroscopy (SERS) has emerged as a powerful technique for probing vibrational signatures of low-dimensional materials such as single-walled carbon nanotubes (SWNTs). We present a plasmonic nanoantenna a design, investigated through the finite difference time-domain (FDTD) simulations. The custom-designed nanoantenna incorporates a bowtie nanoantenna inside a gold ring cavity. This nanostructure offers highly tunable spectral features by adjusting its structural parameters. The proposed design is polarization dependent, and it offers the enhancement of the electric field strength ~ $1.4\times10^8$ for $0^o$ polarization angle. Additionally, we elucidate its performance characteristics for detection of blood and urea samples. The high Raman enhancement factors, providing new avenues for ultrasensitive molecular detection and quantum photonics applications.

**e0014**

**Study on Carbon Removal Uniformity in One Meter Long Capacitive Coupled Plasma Setup Developed for X-ray Mirror Refurbishment**

P. K. Yadav[1,2, a], P. Deep[1], R. K. Gupta[1], S. Gupta[1], and M. H. Modi[1,2]

*[1]Accelerator Physics and Synchrotrons Utilization Division, Raja Ramanna Centre for Advanced Technology, Indore, 452013, India.*

*[2]Homi Bhabha National Institute, Anushakti Nagar, Mumbai 400094, India*

*[a)]Corresponding author: praveenyadav@rrcat.gov.in*

A customized one meter long capacitive coupled RF plasma (CCP) based x-ray mirror cleaning setup is designed and developed. For carbon removal uniformity along 1 meter length, graphitic carbon coated thin film samples deposited on silicon substrates (Si/C) are used. Test samples are exposed to oxygen rf plasma for 4 hours, in steps of 1h, 2h and continuous 4h. After the exposure the samples are characterized by soft x-ray reflectivity (SXR) and x-ray photo electron spectroscopy (XPS) techniques. The SXR measurements indicate that in the first 1h exposure the carbon removal rate is higher, and in the subsequent exposures the carbon removal rate decreases and carbon layer does not remove completely. On contrary, in a 4h continuous exposure, the carbon layer removed completely.

**e0016**

**Structural And Electrical Characterization Of Molybdenum Tri-Oxide Thin Films Deposited On Si (100)**

Abhishek K J [1], Jatindra Kumar Dash [2] and Umananda M Bhatta [1,a)]

*[1] Centre for Incubation,Innovation, Research and Consultancy (CIIRC), Jyothy Institute of Technology, Visvesvaraya University, Tataguni, Off Kanakapura Road, Bengaluru-560082, India.*

*[2] Department of Physics, SRM University- Andra Pradesh, Amaravati 522240, India*

*a) nandasringeri@gmail.com; umananda.b@ciirc.jyothyit.ac.in*

Thin films of Molybdenum were deposited on Si (100) substrate via DC Magnetron sputtering followed by oxidation in air to from Molybdenum Tri-Oxide layers. X-ray diffraction confirmed the formation of $MoO_3$. Scanning Electron Micrographs indicated a smooth-thin layer deposition of $MoO_3$ while Energy dispersive X-ray spectra indicated the presence of Molybdenum, Oxygen and Silicon in the specimen. Electrical characterization of the thin film was performed by taking current-voltage measurements as a function of radiation, voltage and temperature. It was observed that the $MoO_3$ thin films are photosensitive, showed typical semiconductor nature upto 150° C.

**e0017**

**Effect of Annealing on the Structural Properties of Gd/Co Multilayer**

Srijani Haldar[1,2], H. Bhatt[1], P. Gupta[2,3], M. Gupta[4] and Surendra Singh[1, 2,*]

*[1] Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai- 400085, India*

*[2] Homi Bhabha National Institute, Anushaktinagar, Mumbai-400094, India*

*[3] Engineering Applications Lab, Raja Ramanna Centre for Advanced Technology, Indore 452013, India*

*[4] UGC-DAE Consortium for Scientific Research, Khandwa Road, Indore 452017, India*

*Corresponding author: surendra@barc.gov.in*

Strong antiferromagnetic coupling at the interfaces of rare earth (RE)-transition metal (TM) heterostructures gives rise to novel magnetic properties. In addition, the emerging properties arise due to the broken translational and inversion symmetry at the interfaces. Interface structure and morphology tend to play an important role in determining depth dependent structure and magnetic properties of these heterostructures. Annealing of heterostructures and multilayers modify the interface morphology and structure properties. We have studied the effect of isothermal annealing at 300 $^0$C for different time of Gd/Co multilayer and found alloy (GdCo2) formation at the interfaces. The evolution of structural properties of Gd/Co multilayer induced by isothermal annealing in vacuum for different times has been studied by x-ray scattering techniques. Isothermal annealing of the multilayers at 300 ° C for a very short period of 0.5 hours showed a significantly large interdiffusion of atoms between the Gd and Co layers accompanied by formation of polycrystalline $GdCo_2$ alloy phases at the interfaces. Using X-ray reflectivity (XRR) we also estimated diffusion length of the atoms at the interfaces.

**e0018**

**Influence of Structural Evolution on Magnetic and Electrical Response of $Ni_{0.5}Co_{0.5}Fe_2O_4$ Thin Film**

Somnath Sahu, Pamu Dobbidi∗

*Department of Physics, Indian Institute of Technology Guwahati, Guwahati, Assam 781039, India*

*E-mail: pamu@iitg.ac.in*

Ferrite thin films have attracted considerable attention due to their distinctive functional properties, making them promising candidates for advanced electronic and spintronic applications. However, achieving phase-pure growth with a uniform microstructure remains a significant challenge. In this study, $Ni_{0.5}Co_{0.5}Fe_2O_4$ (NCFO) thin film is deposited onto Pt/Si (111) substrates using the pulsed laser deposition (PLD) technique to study the influence of structural evolution on magnetic and electrical leakage characteristics. The deposited films exhibited the formation of a single-phase spinel structure, with dense packed grains with an average surface roughness of approximately 3 nm. Magnetic hysteresis measurements exhibited soft ferromagnetic behavior

with a coercivity of 27 Oe, saturation magnetization of 302 emu/cc, and remnant magnetization of 10 emu/cc. Leakage current measurements revealed low leakage density (~$3.51 \times 10^{-5}$ A/cm²), with conduction dominated by Ohmic behavior at low fields and a transition to space charge limited conduction (SCLC) at higher fields. These results highlight the strong correlation between microstructural features and functional properties, offering insight into the design of NCFO thin films for advanced electronic applications.

**e0019**

**From Coffee Rings to Saucer-shaped Deposits via Reduced Graphene Oxide and Graphene Oxide-laden Aqueous Sessile Droplet Desiccation**

Ravi Kumar Shukla[1], Jitendra Bahadur[2,3], Rajneesh Bhardwaj[4], and Sanghamitro Chatterjee[1,*]
[1]*Advanced Functional Smart Materials Laboratory, Department of Physics, DIT University, Dehradun: 248009, India.*
[2]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai: 400085, India.*
[3]*Homi Bhabha National Institute, Anushaktinagar: 400094, India.*
[4]*Department of Mechanical Engineering, Indian Institute of Technology Bombay, Mumbai: 400076, India.*
**Email:sanghamitro.chatterjee@dituniversity.edu.in*

The aqueous sessile droplet evaporation-assisted colloidal deposits of reduced graphene oxide (rGO) and graphene oxide (GO) is investigated herein. The rGO species exhibits conventional advection with the evaporation-assisted radially outward flows, yielding a classic "coffee-ring" deposit pattern. Intriguingly, the ubiquitous coffee ring pattern is completely suppressed for the case of GO, which results in a uniform deposit pattern that resembles a inverted saucer-like shape. The observed transition stems from the dense oxygen functionality, especially the presence of hydroxyl (O−H) groups on GO the surfaces. First, due to the amphiphilicity, the GO sheets are captured at the liquid-vapor interface. Subsequently, they spontaneously form self-assembled Liquid Crystal (LC) domains brought about by the hydrogen bonding interaction mediated by the local $H_2O$ molecules, as confirmed by Raman spectra. Polarizing Optical Microscopy textures and Small Angle X-ray Scattering (at BL-18 beamline, RRCAT Indore, India) conclusively proved that the formed LC phases are lamellar smectic. As a result of interface capture and self-assembled LC causes the GO sheets to be held together strongly, and they are guided by the descending interface to deposit uniformly onto the underlying surface.

**e0020**

**Mixed Langmuir Monolayers Of 8CB And BHAB**

Shekanna H , Bharat kumar
*Department of Physics, Central University Of Karnataka – 585367, Karnataka, India*
**Email:bharat@cuk.ac.in*

The 8CB molecule (4-cyano-4-n-octylbiphenyl) belongs to a class of liquid crystal compounds, which are designed for specific uses in technologies such as liquid crystal displays, biosensors and other photosensitive devices. Most of these applications involve thin films of mixtures of liquid crystal and photoactive molecules. Hence, it is important to study the properties of 8CB monolayer in the presence of photoactive molecules. In this work we have studied the quasi-2D phases exhibited by the monolayer films of mixtures of 4,4Bis (heptyloxy) azobenzene (BHAB) and 8CB at the air-water interface and analyzed the surface pressure–area per molecule isotherms for understanding the thermodynamic stability of the mixed monolayer.

**e0021**

**Effect of Ag-Doped $V_2O_5$ as an Electron Transport Layer on PM6 Polymer Thin Films for Organic Solar Cell Applications**

Anuradha[1, a] , Rahul Singhal [1] ,Ritu Vishnoi [2]
[1]*Department of Physics , Malaviya National Institute of Technology ,JLN Marg , MalviyaNagar ,Jaipur - 302017, India.*
[2]*Department of Physics, S S Jain Subodh PG College, Jaipur - 302017, India.*
[a)]*Corresponding* author*: 2022rpy9512@mnit.ac.in*

In this study, a thin film of silver vanadium oxide (Ag-$V_2O_5$) was deposited onto a PM6 polymer thin film using radio frequency (RF) sputtering to evaluate its potential as an electron transport layer (ETL) in organic solar cells. Following the deposition, a series of characterization techniques were employed to investigate the structural, optical, and electrical properties of the resulting composite films. UV-Visible spectroscopy revealed a shift in the absorption spectra of the PM6 polymer, indicating strong interaction between the Ag-$V_2O_5$ layer and the underlying polymer PM6. Photoluminescence (PL) spectroscopy showed an increase in PL intensity upon the addition of Ag-$V_2O_5$, indicating reduced non-radiative quenching and suggesting modifications in exciton dynamics at the interface. Raman spectroscopy further confirmed shifts in the characteristic vibrational modes of PM6, supporting the presence of molecular interactions and potential structural modifications resulting from the incorporation of Ag-$V_2O_5$. Scanning Electron Microscopy (SEM) revealed the presence of embedded silver nanoparticles within the polymer matrix, which may contribute to enhanced charge transport pathways. Atomic Force Microscopy (AFM) analysis provided insights into changes in surface roughness and topography induced by the Ag-$V_2O_5$ layer. Additionally, current–voltage (I–V) measurements were conducted to assess the electrical properties of the modified polymer film, demonstrating improved charge carrier mobility and enhanced overall device performance. Collectively, these results suggest that Ag-$V_2O_5$ serves as an effective hole transport layer, significantly improving the optoelectronic properties and performance of polymer-based organic solar cells.

**e0022**

**Investigating The Photoelectrochemical Performance of PLD Synthesized $MoO_3$ Vertical Nanowires**

Shivam Singh, Deepali, Lakshay Bhardwaj, C. M. Vidhya, and J.P. Singh
*Department of Physics, Indian Institute of Technology (IIT) Delhi, Hauz Khas, New Delhi*
*Email: shivam.singh@physics.iitd.ac.in*

Vertically aligned $\alpha - MoO_3$ nanowires were synthesized on FTO substrates using pulsed laser deposition under optimized conditions. Structural and morphological characterizations confirmed phase purity and high aspect ratio, which contributed to enhanced light absorption and charge carrier transport. The nanowire electrodes exhibited a photocurrent density of 2.06 $mA/cm^2$ and a solar-to-hydrogen (STH) efficiency of 2.5%. Mott-Schottky analysis indicated p-type behavior, while EIS and stability tests confirmed efficient charge transfer and good photostability. These findings demonstrate the potential of $MoO_3$ nanowires as efficient photoelectrodes for solar-driven water splitting.

**e0024**

## Room Temperature Non-Volatile Resistive Switching Properties of Vanadium Oxide Thin Film

Koushik Mondal[1], Dip Manna[1], Pawan Kumar Ojha[1], Prashanta Karmakar[2], Supratic Chakraborty[1]
[1]*Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Kolkata 700064, India*
[2]*Variable Energy Cyclotron Centre, 1/AF Bidhannagar, Kolkata 700064, India*
*Email: koushik.mondal1@saha.ac.in

We report fabrication and characterization of a $VO_2$-based metal-oxide-semiconductor (MOS) device exhibiting non-volatile resistive switching behaviour. The devices fabricated on *n*-type Si(100) substrates by depositing $VO_2$ thin film using rf magnetron sputtering exhibit resistive switching with an ON/OFF current ratio of above $10^2$. X-ray photoelectron spectroscopy (XPS) reveals the presence of $V^{4+}$ and $V^{3+}$ associated oxygen vacancies responsible for conductive filament formation. Room temperature *I-V* measurements show a sharp transition from high to the low resistance state (LRS) at around -7 V followed by a RESET to the high resistance state (HRS) in positive cycle confirming non-volatile and reversible switching. These findings highlight the importance of oxygen vacancy dynamics and vanadium redox chemistry enabling resistive switching in $VO_2$-based non-volatile memory devices.

**e0025**

**Electronic property of $Sr_2CoRuO_6$ thin films on LAO(001) and MgO(001) substrates**

Subho Saha, Ram Janay Choudhary
*UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, India*
*Email Id: mesubho.saha@gmail.com*

We probe the substrate induced strain mediated changes in the electronic property of $Sr_2CoRuO_{6-\delta}$ (SCRO) thin films. We have grown thin film of SCRO on LaAlO3 and MgO substrates, where the growth of the thin film is confirmed by x-ray diffraction measurement. XAS measurement shows Co stays in 3+ and Ru remains in 4+ and 5+charge state. Resonant photoemission spectroscopy study reveals that the band near to Fermi level in the valence band is dominated by the hybridized state of Ru with the Oxygen. By comparing the values of onsite coulomb repulsion and charge transfer energy obtained from the combined spectra of VB and conduction band, charge transfer insulating nature of both the thin films of SCRO is established.

**e0026**

**Magnetic Anisotropic Spin-Filtering Tunnel Junction With Ferromagnetic-Insulating Barrier**

Pooja Manral[1], Brij Mohan[1], Tulika Maitra[1], V. K. Malik[1,2a)]
[1]*Department of Physics, Indian Institute of Technology Roorkee, Roorkee-247667, Uttarakhand, India*
[2]*Institute Instrumentation Centre, Indian Institute of Technology Roorkee, Roorkee, 247667, Uttarakhand, India.*
**Email: vivek.malik@ph.iitr.ac.in*

The Study presents a magnetic tunnel junction device that combines highly polarized manganite with a spin-filtering tunnel barrier. The device consists of a thin ferromagnetic insulating barrier for an additional degree of freedom, sandwiched between ferromagnetic manganite electrodes. An investigation on the magneto-transport characteristics of tunnel junctions revealed that these junctions exhibit a hysteretic magnetoresistance that is strongly dependent on the temperature, magnetic field, and its field orientation. The study shows that the switching between resistance states in the tunnel junction is predominantly governed by the magnetization direction within the barrier layer. This behavior arises from the presence of multiple magnetic domain configurations within the device, influenced by the varying coercivity of the films and the intrinsic disorder in the barrier layer. Unlike the sharp transitions typically observed in tunnel junctions, the system undergoes a gradual and continuous reversal of its magnetic moments. This gradual switching introduces a broader and smoother resistance transition, contributing to the round MR loop observed in the experiments. This unique characteristic adding a new dimension to the field of magnetic tunnel junction devices. This study also demonstrates the strong magnetic anisotropy induced by magnetic interfacial coupling.

**e0028**

**Highly Optimized Ag Nanohelix Array for Enhanced SERS-based Biosensing**

Sarjana Yadav[1,2,a], J.P. Singh[1]
[1]*Physics Department, Indian Institute of Technology Delhi, Hauz Khas, New Delhi 110016, India*

[2]*Physics Department, N.R.E.C. College, Khurja, 203131, Chaudhary Charan Singh University, Meerut, India*
[a)]*Corresponding author: yadavsarjana2@gmail.com*
We have fabricated and optimized silver nanohelices (AgNHs) using the glancing angle deposition technique for enhanced SERS performance. The ability of these nanohelices has been investigated using 2-di(4-pyridyl)ethylene (BPE) as the Raman probe. A 2-fold SERS enhancement has been obtained for these substrates in comparison with conventional silver nanorods. The limit of detection (LOD) of BPE using AgNHs has been obtained as $10^{-15}$ M. Further, these substrates are employed to enhance the SERS signal of lab cultured biologically significant bacteria (P. aeruginosa). The formation of high-density 'hotspots' among the AgNHs arrays, along with increased surface area, provides better binding sites and hence entrapment, increasing the net effective contact area between the bacteria and the plasmonic metal surface.

**e0029**

**RF Sputter Grown Thin Film Solid Electrolyte for Advanced Micro-Batteries**

Ananya Bansal[1, a)], Pramod Kumar[1,2] and Ramesh Chandra[1, b)]
[1]*Thin Film Laboratory, Institute Instrumentation Centre, Indian Institute of Technology Roorkee, Roorkee, 247667, India*
[2]*Advanced Technology Institute, University of Surrey, Guildford GU2 7XH, United Kingdom*
*Corresponding author: [a)]ananya_b@ic.iitr.ac.in , [b)]Ramesh.chandra@ic.iitr.ac.in*
Lithium aluminum titanium phosphate (LATP), a NASICON-type oxide, has emerged as a promising solid-state electrolyte due to its high lithium-ion conductivity, wide electrochemical stability window, and compatibility with lithium metal. In this study, dense LATP thin films were successfully deposited using radio frequency magnetron sputtering, a scalable and controllable physical vapor deposition technique. A stoichiometric LATP ceramic target was employed, and deposition parameters such as power, substrate temperature, working pressure, and argon–oxygen gas ratio were optimized to achieve phase-pure, uniform films. Electrochemical impedance spectroscopy performed on Au|LATP|Au symmetric cells demonstrated promising in-plane ionic conductivity in the range of $10^{-4}$ to $10^{-6}$ S·cm$^{-1}$ at room temperature, with low electronic conductivity. These results highlight the suitability of RF-sputtered LATP films for integration into next-generation thin film batteries and microelectronic energy storage systems. The study demonstrates the potential of sputtering-based fabrication as an effective route for producing high-quality, scalable solid-state electrolyte films for solid-state battery applications.

**e0030**

**Fabrication of crystalline silicon-on-insulator structure using ultra-low pressure thermal CVD**

Monika Dhiman[1,*] and Arup Samanta[1, 2]
[1]*Quantum/Nano-Science and Technology Laboratory, Department of Physics, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand, India*
[2]*Centre for Nanotechnology, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand, India*
**Email: monika@ph.iitr.ac.in*
With the increasing demand for high-performance silicon platforms, the direct integration of crystalline silicon thin films on insulator substrates is of growing interest for next-generation electronic and photonic devices. However, conventional methods for achieving crystalline layers on $SiO_2$ involve complex epitaxial growth or wafer bonding processes. In this study, we demonstrate a simplified and scalable approach for the deposition of crystalline silicon thin films on thermally grown $SiO_2$/Si substrates using ultra-low-pressure thermal chemical vapor deposition. The silicon films were synthesized via the pyrolytic decomposition of hydrogen-diluted silane gas at high temperature. Uniform film depositions were verified using field emission scanning electron microscopy. High-resolution transmission electron microscopy, Raman spectroscopy, and high-resolution X-ray diffraction (ω-scan) collectively confirmed that the silicon thin film on $SiO_2$ substrate exhibits a single-crystalline phase. Hence, this process offers a cost-effective and controllable route for fabricating high-quality crystalline silicon thin films on insulator substrates, potentially enabling advanced device integration on standard silicon platforms.

**e0031**

**Influence of Annealing Temperature on Structural, Optical, and Dielectric Properties of PLD-grown $Ba_{0.5}Sr_{0.5}TiO_3$ Thin Films**

VijayaLakshmi Talasila[1, 2] and Venkaiah Malapati[2*]
[1]*Department of Physics, AV College of Arts, Science & Commerce, Hyderabad, Telangana, India*
[2]*Department of Physics, School of Applied Sciences & Humanities, Vignan's Foundation for Science, Technology and Research, Vadlamudi, Guntur, Andhra Pradesh, India*
**email: drvm_sh@vignan.ac.in*
$Ba_{0.5}Sr_{0.5}TiO_3$ (BST) thin films were deposited on n-type Si and quartz substrates using the pulsed laser deposition (PLD) technique. Post-deposition annealing was performed at various temperatures, to optimize the structural and functional characteristics of the films. X-ray diffraction analysis verified the formation of a single-phase cubic perovskite structure. Field emission scanning electron microscope showed a densely packed microstructure, while optical measurements indicated a wide band gap. The dielectric constant measured across varing temperatures remained stable for the film annealed at 700$^o$C. These findings highlight a significant influence of annealing temperature on both structural and dielectric characteristics, confirming the material's potential for use in advanced capacitor technologies.

**e0032**

**When Electrons Paint: Correlation between Local Bonding and Color Revealed for Ti(1-x)Al(x)N Thin Films**

Priti Vishwakarma[1,4], Sumit Kumar [2,3,a)], S.K. Sinha[1], Umesh Mhatre[4,b)]
[1]Birla Institute of Technology, Mesra, Jharkhand - 835215, India
[2]*Radioanalytical Chemistry Division, Bhabha Atomic Research Centre, Mumbai – 400085, India*
[3]*Homi Bhabha National Institute, Mumbai - 400094, India*
[4]*Surface Modification technologies Pvt. Ltd., Mumbai-401208, India*
[a),b)]*Email: sumitk@barc.gov.in; umeshm@smt.co.in*

In this study, we investigate the correlation between the local electronic structure and optical properties of arc-deposited $Ti_{1-x}Al_xN$ thin films prepared with varying aluminum concentrations (x = 15%, 30%, and 50%). X-ray absorption near edge structure (XANES), was employed to probe the local electronic structure, while surface color and the optical band gap were obtained from CIEL*a*b spectroscopy and diffuse reflectance spectroscopy (DRS), respectively. The band gap values were found to increase with Al content up to 30% (2.74 eV at x = 0.15, to 3.7 eV at x = 0.30) and saturated at 3.66 eV for x = 0.50. Additionally, CIEL*a*b analysis reveals a systematic color transition from golden to reddish to purplish with increasing Al. This color variation is attributed to changes in the local electronic structure, as revealed by XANES analysis. XANES composition-dependent changes in shape and peak intensity reflect alteration in unoccupied density of states. Moreover, a consistent shift of the high-energy spectral features toward lower energies with increasing Al content further supports the evolution of the local bonding environment, which influences the electronic structure and, consequently, the optical appearance of the films.

**e0035**

**One-step NiO/Ni Nano Heterostructures Formation in Microwave Synthesis and Enhanced Ammonia Gas Sensing Response**

Upesh Kumar Appikonda[1)], and Paramesh Gadige [1), a)]
*Department of Physics, Sri Sathya Sai Institute of Higher Learning, Prashanthi Nilayam Campus, Puttaparthi, 515134, Andhra Pradesh, India*
**Corresponding author: gadigeparamesh@sssihl.edu.in*

p-type semiconducting nickel oxide (NiO) and its heterostructures have been explored for gas sensing due to their interesting properties, which are tunable by different strategies. This study presents gas sensing studies on NiO/Ni nano heterostructures formed through one step microwave synthesis and comparison with the conventional annealing process. X-Ray diffraction characterization confirms the NiO/Ni heterostructures with a large Ni phase fraction in the microwave route compared to the conventional annealing process. Moreover, heterostructure thin films are formed on silicon substrates with two point electrodes for gas sensing studies, where the changes in the resistance are monitored by exposing to different gas concentrations (acetone, ethanol, methanol, ammonia, and propanol). The highest gas selectivity and enhanced sensing response for ammonia is obtained for microwave processed NiO/Ni heterostructures. This is attributed to the NiO/Ni (semiconductor-metal) nano heterostructure phenomena, catalytic activity and enhanced charge transfer due to high Ni fraction.

**e0036**

**The Effect of Oxygen Vacancy and Phase Transition on Dielectric Properties of $HfO_2$ Thin Films**

Mangla Nand[1, *], Partha Sarathi Padhi[2,3], Shilpa Tripathi[1,4], Yogesh Kumar[1], Pankaj Misra[3,4] and S. K. Rai[5]
[1]*Beamline Development and application Section, Bhabha Atomic Research Centre, Mumbai-400085*
[2]*Department of Solid State Sciences, Ghent University, Conformal Coating of Nanostructures (CoCooN), Krijgslan 281 S1, B-9000 Ghent, Belgium*
[3]*Oxide Nano Electronics Lab., Laser Material Processing Division, Raja Ramanna Centre for Advanced Technology, Indore, Madhya Pradesh 452013*
[4]*Homi Bhabha national Institute, Anushaktinagar, Mumbai,Maharashtra,- 400094*
[5]*Accelerator Physics and Synchrotrons Utilization Division, Raja Ramanna Centre for Advanced technology, Indore, Madhya Pradesh-452013*
**Email:kappu001@gmail.com*

Undoped and Y-doped $HfO_2$ thin films were fabricated on Si(100) and platinized Si substrates using pulsed laser deposition system. Structural and compositional analysis (TEM, GIXRD) revealed a phase transition from monoclinic to cubic with increasing Y content. Dielectric and electrical properties, evaluated using Pt-based MIM capacitors, showed an increase in dielectric constant from ~24 to 38 as Y doping increased from $x = 0$ to 0.20 in $Hf_{(1-x)}Y_xO_2$ films. However, increased Y doping also led to higher leakage current density (~$2.6 \times 10^{-5}$ to $5.3 \times 10^{-3}$ A/cm$^2$ at 1 V), attributed to enhancement of Y-induced oxygen vacancies confirmed by XPS and phase transformation. These results establish a clear correlation between structure and electrical properties in Y-doped $HfO_2$ films, highlighting their potential for electronic applications.

**e0037**

**Investigation of Interface Compounds and X-ray Optical Performance of Ultra-Low Thickness WC/SiC, WC/Si, W/SiC, and W/C/Si Multilayers**

Simran Atwal1, [2*], K Bhattacharyya[2,3], Pooja Gupta[4], S Rai[4], D Bhattacharyya1, 2, A Biswas[1, 2,]

[1]*Atomic and Molecular Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, INDIA*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai-400094, INDIA*
[3]*Chemistry Division, Bhabha Atomic Research Centre, Mumbai-400085, INDIA*
[4]*Indus Synchrotron Utilization Section, Raja Ramanna Centre for Advanced Technology, Indore- 752013, INDIA.*
**Email: simiatwal@barc.gov.in*

In X-ray multilayer optics, material selection and interface engineering are critical for maximizing reflectivity. Recent studies have shown that introduction of a carbon buffer layer at the W/Si interface enhances the X-ray supermirror performance by forming interfacial carbide compounds. In this work, we compare the X-ray optical performance of carbide-based multilayers: WC/SiC, WC/Si, W/SiC, and W/C/Si. 10 bi-layer structures with periodic thicknesses of 12–21 Å were deposited using ion beam sputtering. Grazing Incidence X-ray Reflectivity (GIXR) measurements revealed that W/SiC exhibits a nearly flat Scattering Length Density (SLD) profile at lower thicknesses, indicating strong interdiffusion. Further comparison using 75 bi-layer samples showed that WC/Si performs best for Bragg peaks ~6°, while WC/SiC is superior around 4°. These results are supported by X-ray photoelectron spectroscopy (XPS) analysis, which confirmed that the chemical properties of the interface support the observed reflectivity trends.

**e0039**

**Effect on photolumienecence property of graphitic carbon nitrate and zinc oxide nanocomposite**

P. Kumar[1], D. Banerjee[2], A. K. Sharma[3]
[1,2,3] Thin Film and Nanotechnology Laboratory, Department of Physics, Faculty of Engineering and Computing Sciences,
*Teerthanker Mahaveer University, Moradabad, UP 244001, India*
*Corresponding Author: drdiptonil.engineering@tmu.ac.in , nilju82@gmail.com*

The present work represents the graphitic carbon nitride (GCN) and Zinc Oxide (ZnO)-based nanocomposite, which have attracted significant attention due to their enhanced photoluminescence (PL) properties and potential optoelectronic applications. The GCN-ZnO nanocomposite was synthesized via a simple wet chemical method to investigate the effect of composite formation on PL behavior. The PL spectra reveal indicating strong interfacial interaction and charge transfer between the two components. The spectrum showed different peaks related to defect-related transitions and trap states, with CIE coordinates confirming blue-cyan emission. These findings suggest that GCN-ZnO nanocomposites offer a tunable platform for photonic and sensing applications.

**e0040**

**Binary and ternary silver phosphate-based hybrids for SERS detection of Raman reporter molecules**

Fadeela Chundekatt Ummer [1, a] Nandakumar Kalarikkal [1, 2, 3, b]
[1]*International and Inter University Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University, Kottayam-686560, Kerala, India*
[2]*School of Pure and Applied Physics, Mahatma Gandhi University, Kottayam-686560, Kerala, India*
[3]*International Centre for Ultrafast Studies, Mahatma Gandhi University, Kottayam-686560, Kerala, India*
*Email: [a)] nkkalarikkal@mgu.ac.in [b)] cufadeelah@gmail.com*

In this work, we systematically investigated the structural and optical properties of binary and ternary hybrids of silver phosphate for SERS applications. The hybrids are grown in situ method using wet chemical synthesis. The binary hybrid consists of silver and silver phosphate and the ternary hybrids consists of silver, silver phosphate and graphene oxide. The hybrids are characterized using UV-Visible spectroscopy, FT-IR spectroscopy, XRD, FE-SEM and XPS analysis. SERS studies were performed using confocal Raman spectrometer using 532 nm wavelength.

**e0041**

**Thickness-Dependent Thermoelectric Enhancement in BSTS Thin Films: Role of Surface States and Dimensionality**

Vishnu Sharma and Sandip Chatterjee
[1] *Indian Institute of Technology-BHU Varanasi*
**Email: schatterji.app@iitbhu.ac.in*

We report the structural and thermoelectric characterization of Bi-Sb-Te-Se (BSTS) thin films with thicknesses of 20 nm and 35 nm, grown via pulsed laser deposition (PLD), and compare them with bulk BSTS samples. X-ray diffraction (XRD) confirms that the films are highly oriented along the c-axis with dominant (00l) reflections. Temperature-dependent resistivity measurements reveal a crossover from semiconducting to metallic behaviour with decreasing film thickness, highlighting enhanced surface conduction in thinner films. The Seebeck coefficient (S) increases significantly in the thin films, achieving values exceeding 600 μV/K at 300 K for 20 nm films, surpassing bulk BSTS. The combined high S and moderate resistivity indicate improved thermoelectric performance in ultrathin BSTS films. These results underscore the role of quantum confinement and surface states in enhancing thermoelectric efficiency.

**e0042**

**Fractal Surface Engineering of NiO Thin Films for Enhanced Ag/NiO/FTO Schottky Diode Properties**

Pooja Redhu[1], Monika Shrivastav[1], Chandra Kumar[2], Sanjeev Kumar[1*]
[1]*Department of Physics, University Institute of Sciences, Chandigarh University, Mohali-140413, Punjab, India*
[2]*Escuela de Ingeniería, Facultad de Ciencias, Ingeniería y Tecnología, Universidad Mayor, Santiago 7500994, Chile*
**Corresponding author: Sanjeev Kumar (sanjeev.uis@cumail.in)*

NiO thin films are promising p-type semiconductors owing to their high optical transparency, wide bandgap, and elevated work function, making them suitable for optoelectronic and photovoltaic applications. In this study, NiO thin films were sputter-deposited on FTO substrates prepared via metal-assisted chemical etching and the influence of fractal surface morphology on their optical and electrical properties was systematically investigated. Atomic force microscopy (AFM) and fractal analysis revealed that air annealing induces a progressive evolution of the surface morphology from a relatively smooth profile to a more self-affine, scale-invariant texture. The extracted fractal dimension ($D_f$) exhibited a strong correlation with surface roughness metrics, indicating enhanced topological complexity. This increase in fractal dimensionality is directly associated to enhanced photon trapping, diffuse light scattering, and disorder-related sub-band states, thereby modifying the optical response of the NiO films. On the electrical properties, the Ag/NiO/FTO Schottky diodes exhibited modified charge transport behaviour as a function of surface fractality. I–V characteristics analyzed through thermionic emission theory, Cheung's method, and Norde's function revealed that increased fractal dimension led to a decrease in effective barrier height and a rise in the ideality factor, indicative of enhanced interface recombination and tunnelling-assisted transport. The fractal surface effectively increased the density of active interface states and local electric field variations, promoting non-uniform current paths and impacting carrier injection dynamics. Collectively, these findings underscore that fractal surface morphology is not merely a geometric feature but a fundamental parameter that modulates both the optical absorption mechanism and the electrical transport phenomena in NiO-based Schottky barrier devices. This insight opens new possibilities for engineering surface fractality as a tunable design parameter in optoelectronic devices.
**Keywords:** Sputtering, Fractal Dimension, AFM, Thin Films, Optical Properties, Schottky Diode

**e0043**

**Structural Analysis of Sputtered $MoS_2$ Film Leading to the Superlubricity**

Sanat Kumar and Rishi Sharma*
*Department of Physics, Birla Institute of Technology, Mesra, Ranchi, Jharkhand-835215, India*
**Email: rishisharmabit@hotmail.com; rsharma@bitmesra.ac.in*

Molybdenum disulfide ($MoS_2$) is a well-known solid lubricant, widely utilized in tribological applications due to its layered structure and low shear strength covalently bonded S–Mo–S trilayers held together by weak van der Waals forces. This anisotropic bonding facilitates easy shear between basal planes, enabling low friction during sliding. In this study, pure $MoS_2$ thin films were deposited on silicon substrates using radio frequency (RF) magnetron sputtering under controlled vacuum conditions. Structural characterization was carried out using X-ray diffraction (XRD), Raman spectroscopy to assess crystallinity and phase purity. The XRD patterns confirmed the hexagonal 2H-$MoS_2$ phase with preferential (002) orientation, indicating alignment of the basal planes parallel to the substrate—an essential feature for optimal tribological performance, while Raman spectra revealed prominent $E_{2g}$ and $A_{1g}$ modes, indicating good structural integrity and characteristic of well-ordered 2H-$MoS_2$. The integrity and orientation of these crystalline planes play a critical role in reducing friction by promoting interlayer slippage. This study underscores the importance of structural ordering and phase purity in tailoring $MoS_2$ as an effective solid lubricant in ambient environments.

**e0044**

**Optimization of Thickness Uniformity of Multilayer Thin Films Deposited by Magnetron Sputtering on Curved Substrates Using Planar and Cylindrical Magnetron: Simulation and Experimental**

Ravit Pulyani[1]*, S K Ghosh[2], D Bhattacharyya[3,4], A Biswas[3,4]
[1]*Department of Physics, Indian Institute of Technology, Roorkee, Uttarakhand – 247667, INDIA*
[2]*Material Processing & Corrosion Eng. Division, Bhabha Atomic Research Centre, Mumbai-400085, INDIA*
[3]*Atomic and Molecular Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, INDIA*
[4]*Homi Bhabha National Institute, Anushaktinagar, Mumbai-400094, INDIA*
**Email: ravitp28@gmail.com*

Deposition of multilayer thin films is critical for the development of advanced optical devices, including space-based X-ray telescopes. In this study, sputtered deposition profiles of Ti were simulated using the Monte-Carlo techniquebased simulation software SiMTRA, for both rectangular and cylindrical magnetrons. The deposition behavior was analyzed on planar and curved substrates under varying chamber pressures and target-to-substrate distances. Optimal deposition conditions were identified, achieving film thickness uniformity within ±0.25%. Furthermore, Ti and 10 bi-layer periodic (Ni/Ti) multilayer films were deposited on curved substrates using a large area DC magnetron sputtering system. Grazing Incidence X-ray Reflectivity (GIXR) measurements confirmed a thickness uniformity of ±1.8% on a curved surface with a 70 mm radius of curvature and 130 mm width—comparable to the geometry used in NASA's NuSTAR space telescope.

**e0045**

**Influence of Layer Thickness on the Crystalline and Optical Characteristics of Mg-Doped ZnO Films for UV Applications**

Sunena Subhash and Sudheendran Kooriattil
*Department of Physics, Sree Kerala Varma College, Thrissur, University of Calicut, Kerala – 680011, India*
**Email: sunenamidhunam827@gmail.com*

Mg-doped ZnO ($Zn_{0.85}Mg_{0.15}O$) thin films were prepared on silicon (Si) substrates by the sol-gel spin coating method to examine the effect of film thickness on their structure, morphology, and optical properties. X-ray diffraction established the wurtzite structure with dominant c-axis orientation. Cross-sectional SEM images and surface SEM images indicated uniform growth and increasing agglomeration with an increase in thickness. UV–Vis spectra reported high transmittance with a clear cut-off in the UV

region, whereas Tauc plots revealed thickness-dependent red shift in the optical band gap from 3.364 eV to 3.275 eV. The findings demonstrate the promise of thickness-regulated Mg-doped ZnO films for optoelectronic and UV-transparent device technology.

**e0046**

**Effect of C and $^{11}B4C$ in improving interface quality of polarizing Fe/Si Multilayer Neutron Optics**

P. Sarkar[1], N. Ghafoor[2], A. Biswas[1], D Bhattacharyya[1], Sophia Sahoo[3], J. Birch[2], F. Eriksson[2]
*[1] Atomic & Molecular Physics Division, Bhabha Atomic Research Centre, Mumbai, 400 085, India, [2]Thin Film Physics Division, Department of Physics, Chemistry and Biology (IFM), Linköping University, SE-581 83 Linköping, Sweden, [3]MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, NE*
**Email: piyali.sarkar4@gmail.com*

Fe/Si-based supermirror polarizers are vital in polarized neutron optics due to their high reflectivity and spin selectivity. However, their performance is limited by interface imperfections, including roughness, interdiffusion, and silicide formation. This study explores the effect of incorporating carbon (C) and boron carbide ($^{11}B_4C$) into Fe/Si multilayers using ion-assisted magnetron sputtering. Structural characterization reveals that both additives promote amorphization, suppress crystallinity, and reduce interface diffusion. Grazing incidence X-ray absorption spectroscopy (XAS) measurements confirm reduction in silicide formation, while polarized neutron reflectivity simulations and magnetometry measurements show improved spin reflectivity and polarization. These findings suggest C and $^{11}B_4C$ as effective additives for enhancing the performance of Fe/Si neutron optical devices.

**e0047**

**Magneto-Transport and Spin-Polarized Tunneling in Polycrystalline $La_{0.67}Ca_{0.33}MnO_3$ Thin Films**

Brij Mohan[1], Pooja Manral[1], Mayank Nautiyal[1], V. K. Malik[1,*]
*[1]Department of Physics, Indian Institute of Technology Roorkee, Roorkee – 247667, India*
**Email: vivek.malik@ph.iitr.ac.in*

The low-field magnetoresistance behavior of polycrystalline $La_{0.67}Ca_{0.33}MnO_3$ (LCMO) thin films deposited on various substrates has been systematically investigated. X-ray diffraction analysis confirms the polycrystalline nature of the films. Magneto-transport measurements reveal a pronounced reduction in electrical resistance across the entire temperature range below the insulator-to-metal transition temperature, particularly when the magnetic field is applied parallel to the film surface, as compared to the perpendicular configuration. Furthermore, resistance as a function of magnetic field exhibits distinct positive magnetoresistance peaks at temperatures below the transition point. These peaks correspond closely to the coercive field of the respective samples. The observed magnetoresistive behavior is primarily attributed to spin-polarized tunneling across grain boundaries.

**e0049**

**Effect of Molecular Weight of DPP-DTT on Microstructural Ordering and Charge Transport**

Suman Kumar Ghosh*, Souvik Jana, and Satyajit Hazra
*Saha Institute of Nuclear Physics, A CI of HBNI, 1/AF Bidhannagar, Kolkata 700064, India*
**Email:sumankumar.ghosh@saha.ac.in*

This work explores the influence of molecular weight on the microstructural ordering and charge transport properties in DPP-DTT thin films. Thin films derived from two molecular weights under identical processing condition, were investigated using X-ray reflectivity, optical absorption spectroscopy, atomic force microscopy, and electrical transport measurement. Films prepared from the lower molecular weight polymer exhibited superior out-of-plane ordering, distinct vibronic features in optical absorption, and wider grains in topography suggesting more ordered chain packing which can be attributed to higher diffusivity and regioregularity of low molecular weight polymer chains. In contrast, the higher molecular weight polymer films showed poor ordering, narrower grains, and broad, featureless spectra in optical absorption. Consistent with these observations, OFET devices based on the low molecular weight polymer demonstrated significantly higher mobility. These findings highlight the critical role of molecular weight in determining device performance.

**e0050**

**Influence of Energy and Temperature of Dielectric Surface on Growth and Performance of Ph-BTBT-10-based OFETs**

Souvik Jana[a)], Suman Kumar Ghosh and Satyajit Hazra
*Saha Institute of Nuclear Physics, A CI of HBNI, 1/AF Bidhannagar, Kolkata 700064, India*
**Email:*souvik.jana@saha.ac.in

The combined effect of temperature and energy of the dielectric surface on the growth, morphology and charge transport properties of physical vapor deposited Ph-BTBT-10 bilayer (~4 nm) films have been investigated. On bare $SiO_2$ substrates, vertical ordering and domain size of Ph-BTBT-10 improve with substrate temperature leading to an excessive domain separation at 100°C, disrupting connectivity. In contrast, OTS-treated $SiO_2$ substrates promote edge-on bilayer ordering even at room temperature. However, limited domain growth and reduced interconnectivity at elevated temperatures hinder the charge transport. Our results highlight that critical balance of molecular orientation, domain size, and inter-domain connectivity, governed by the interplay between the thermal-energy and surface-energy of the dielectric, is the key requirement for proper charge transport.

**e0051**

**Metal-Organic interphase layer formation probed by Hard X-ray Photoelectron Spectroscopy at PES beamline, Indus-2**

Jaspreet Singh*, Uday Sule, R K Sharma and Jagannath
*Technical Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, India.*
**Corresponding author: jaspreet@rrcat.gov.in*
In the present paper, we present the study of metal-organic interface in aluminium (Al) and magnesium phthalocyanine (MgPc) multilayer stack on Si substrate surface using hard x-ray photoelectron spectroscopy (HAXPES). A broad interface layer of thickness ~ 1.54 nm was formed when aluminium was vacuum evaporated on pre-deposited MgPc thin film (Al-MgPc) on Si substrate. The broad interface layer in Al-MgPc sample was observed due to the diffusion of thermally activated aluminium atoms in soft and open matrix of pre-deposited MgPc thin films.

**e0052**
**Influence of Ruthenium Refractory Metal Interface on Magneto-Structural Properties of CoFeB Alloy Thin Films**
Momin[1,2], Shainky Rana[1], Mukul Gupta[3] , S.K.Rai[1,2] and Pooja Gupta[1,2, a)]
*[1]Raja Ramanna Centre for Advanced Technology, Indore 452013, India*
*[2]Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400094, India*
*[3]UGC-DAE Consortium for Scientific Research, Khandwa Road, Indore 452017, India*
**Email: pooja@rrcat.gov.in*
This study investigates the influence of a Ruthenium (Ru) interface on the structural and magnetic properties of magnetron-sputtered CoFeB thin films. A series of single-layer CoFeB films (5–50 nm) and Ru/CoFeB(25 nm)/Ru trilayers were synthesized and characterized using X-ray reflectivity (XRR), grazing incidence X-ray diffraction (GIXRD), magneto-optical Kerr effect (MOKE), and vibrating sample magnetometry (VSM). The CoFeB layers maintained an amorphous structure and exhibited soft magnetic properties with uniaxial magnetic anisotropy (UMA) for the deposited thickness range. Insertion of Ru buffer enhances saturation magnetization (~1568 emu/cm³) and reduces coercivity (~34 Oe), while preserving the amorphous structure. UMA remained unaffected by Ru thickness variation. These findings highlight the efficacy of Ru buffering in tuning CoFeB-based magnetic heterostructures for spintronics and memory applications.

**e0053**
**Quasiperiodic Ga Monolayer on *i*-Al-Pd-Mn Surface**
Pramod Bhakuni[§], Sudipta Roy Barman[a)]
*UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, Madhya Pradesh, India*
**Email: [a)]barmansr@gmail.com, [§]bhakuni.pramod188@gmail.com*
In this study, we employ scanning tunneling microscopy to demonstrate the presence of quasiperiodicity in elemental Ga adlayer grown on a fivefold icosahedral Al-Pd-Mn quasicrystal at low temperature. STM topographies reveal the formation of distinct quasiperiodic motifs such as $\tau$-GaWF and ring motifs, indicative of quasiperiodic ordering. Moreover, the Fourier transform of these real-space images displays sharp tenfold spots, confirming the presence of quasicrystalline order. Low-energy electron diffraction measurements also demonstrate the presence of fivefold symmetry in the Ga monolayer.

**e0054**
**Interplay of Light-Element Interstitials and Spin Transport in Transition Metal Epitaxial Thin Films**
Nitipriya Tripathi[1*], Shrawan Kumar Mishra[1], and Shinji Isogami[2]
*[1]School of Materials Science & Technology, IIT (BHU), Varanasi, India.*
*[2] Research Centre for Magnetic and Spintronics Materials, NIMS, Japan*
*Email: *nitipriyatripathi.rs.mst20@iitbhu.ac.in*
The integration of light-element interstitials such as nitrogen, boron, and carbon into transition metal systems has opened new avenues in solid-state physics, particularly in controlling magnetic and spin transport phenomena. This work investigates the epitaxial growth and physical properties of transition metal-based thin films, primarily $Mn_3PtN$, and compares them with the controlled sample $Mn_3Pt$. We focus on how interstitial defects and ordering modulate structural, magnetic, and spin-current conversion efficiencies. In $Mn_3PtN$, nitrogen vacancies are shown to induce significant changes in spin transport responses, highlighting the positive effect of nitrogen. Our findings provide fundamental insights into the coupling between lattice structure, electronic configuration, and spin dynamics, offering a pathway toward designing spintronic materials with low environmental impact and tunable functionalities.

**e0055**
**Quasiperiodic Potassium adlayer on fivefold Al-Pd-Mn surface**
Vipin Kumar Singh[§,*], Pramod Bhakuni, and Sudipta Roy Barman[#]
*UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, Madhya Pradesh, India*
**Present affiliation: CSIR- CSIR-Central Glass and Ceramic Research Institute, 196 Raja S.C. Mullick Road, Jadavpur, Kolkata-700032.*
*Email: #barmansr@gmail.com, §svipin65@gmail.com*
Quasiperiodicity of potassium (K) monolayer on the five-fold surface of icosahedral Al-Pd-Mn (*i*-Al-Pd-Mn) is demonstrated using scanning tunneling microscopy (STM) and low energy electron diffraction (LEED). Atomically resolved STM images reveal the

formation of distinct quasiperiodic pentagonal motifs that resemble, but are larger than, the white flower motifs of *i*-Al-Pd-Mn. The quasiperiodicity of the K monolayer is confirmed by Fourier transform of the STM image and the LEED pattern.

**e0056**

**Defect Engineering in ZnO using Nitrogen Ion Irradiation**

V. S. Ghemud[1,2], Priya Jadhav[1,3], Priyanka Kolhe[1,4], Pandit Shelke[3] and Shailendra Dahiwale[2*]
*[1] Department of Physics, BJS's Arts, Sciecne and Commerce College, Pune 412207.*
*[2]Department of Physics, Savitribai Phule Pune University, Pune 411007,*
*[3]Department of Physics, PDEA's Baburaoji Gholap College, Pune 411027,*
*[4]Department of Physics, J.S.P.M. University, Pune 412207.*
**Corresponding author: shailsd@gmail.com*

The ZnO thin films were synthesized by chemical bath deposition (CBD) method and further irradiated by low energy nitrogen ions with different fluence. The structural, morphological and optical properties of the pristine and irradiated films have been investigated using X-ray diffraction (XRD), Raman spectroscopy, scanning electron microscopy (SEM) and UV-VIS Spectrophotometer. The X-ray diffraction analysis shows that the films are polycrystalline with hexagonal structure and the confirmation of structural formation is provided by Raman spectra. It also reveals the oxygen vacancy type point defects have been introduced by ion irradiation. Upon irradiation it is seen that the absorbance also shift towards visible region, suggesting its enhanced application in optoelectronics, while oxygen vacancy formation promotes its gas-sensing application.

**e0057**

**Effect of Annealing on the Properties of Electrodeposited InSb Thin Films**

Joginder Singh*
*Noida Institute of Engineering and Technology, Greater Noida India- 201310*
*E-mail:* jogindersingh@niet.co.in

Indium antimonide (InSb) thin films were successfully grown on stainless-steel substrates by DC electrodeposition. Elemental analysis showed the deposited films consisted of 51.9% indium and 48.1% antimony. X-ray diffraction (XRD) studies revealed the films to be polycrystalline with a predominant (111) orientation. Key structural parameters, including crystallite size (D), dislocation density (δ), and strain (ε), were evaluated. The crystallite size increased with annealing temperature, ranging from 61.64 nm to 66.27 nm. Raman spectroscopy confirmed the presence of the transverse optical (TO) phonon mode, indicating the crystalline nature of the electrodeposited films.

**e0058**

**Effect of swift heavy Ion irradiation on spin coated $SnO_2$ Thin films.**

Anil Gome [1*], Fouran Singh[2] ,V. Ganesan[1], V.Raghavendra Reddy[3] and R.Venkatesh[3]
*[1]Medicaps University, A.B. Road, Pigdamber, Rau Indore 45333, India.*
*[2]Inter University Accelerator Centre (IUAC), New Delhi 110067, India*
*[3]UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore 452001*
**Corresponding Author: anugome@gmail.com*

In the present work we investigate the effects of swift heavy ion Au $^{+9}$ (SHI) irradiation on $SnO_2$ thin films, focusing on changes in structural, electronic and morphological properties. $SnO_2$ Thin Films are coated on a silicon substrate using the sol-gel method and films were dry on 70°C which further irradiated with 120MeV $Au^{+9}$ ions with different ion fluence. Glancing angle x ray diffraction (GIXRD) is taken to probe the structural study of films. Data shows broad peaks amorphous structure which is transformed to β- Sn Phase as increasing the ion fluence. To probe the electronic properties of films we used Mossbauer spectroscopy, results confirms change in oxidation state of $SnO_2$ film ($Sn^{+4}$) converts to SnO-βSn ($sn^{+2}$). By tuning these electronic properties might be useful for various practical applications.

**e0060**

**Sputtering Power Mediated Growth Dynamics in Scandium Doped Aluminum Nitride (AlScN) Thin Films**

Sivaprasad Warrier U L[1], Sandeep Sanjeeva [1], Jyothilakshmi R [1], P. Poornesh [2], Kodihalli K Nagaraja [1*]
*[1]Alternative Energy Materials Laboratory (AltEMate Lab), Department of Physics, Manipal Institute of Technology (MIT), Manipal Academy of Higher Education (MAHE), Manipal, India – 576104*
*[2]Laser and Non-linear Optics Laboratory, Department of Physics, Manipal Institute of Technology (MIT), Manipal Academy of Higher Education (MAHE), Manipal, India – 576104*
*Email: * nagaraja.kk@manipal.edu*

This study examines the effect of total sputtering power on Aluminum Nitride (AlN) thin films doped with a fixed 30% Scandium (Sc) composition to Al sputtering power, aiming to clarify Sc incorporation into the AlN lattice. X-ray diffraction (XRD) shows crystallinity depending on deposition rate, which rises with higher power, while substrate temperature critically affects structure. SEM and AFM analyses reveal increased grain agglomeration at higher powers, linked to film thickness growth from 0.8 μm to 2 μm and surface roughness from 5 nm to 10 nm. AFM confirms that power variations drive morphological evolution. Energy Dispersive X-ray Spectroscopy (EDS) shows uniform Sc distribution with a stable 18 % across all samples. IV measurements indicate high film quality, with low leakage current of $10^{-9}$ A even at 10 V DC for best sample. The findings provide insights into

the relationship between deposition parameters and microstructure, enabling more controlled fabrication of high-quality AlScN thin films for advanced device applications.

**e0062**

**Annealing-Driven Modulation of Nonlinear Optical Characteristics in $TiO_2$ Thin Films**

Romita Chouhan[1,a], Arpana Agrawal[2], Pratima sen[3]
[1]*Shri Govindram Seksaria Institute of Technology and Science, Indore, India*
[2]*Shri Neelkantheshwar Government Post-Graduate College, Khandwa, India*
[3]*Laser Bhawan, School of Physics, Devi Ahilya University, Khandwa Road, Indore- 452001, India,*
[a)]*Corresponding author:romitachouhan15@gmail.com*

In the present article, nonlinear optical characteristics of $TiO_2$ thin film have been investigated. The DC magnetron sputtering technique was used to deposit the film in an argon and oxygen mixture. The grown film was post-annealed at two distinct temperatures. Crystalline properties of the films are investigated using the X-ray diffraction technique, which exhibits the crystalline character of the film up on annealing. From the UV-Vis spectra, we observed that the band gap value reduces for the film annealed at higher temperature. The Intensity-dependent nonlinear optical properties of the film are obtained using the z-scan technique in open and closed aperture geometry, from which we have obtained the nonlinear absorption coefficient as well as the nonlinear refraction coefficient and also observed the effect of annealing temperature on it. The larger nonlinear response of the film has drawn its utility in different optoelectronic devices.

**e0063**

**Depth-resolved study of interface magnetism in Rubrene/$^{57}$Fe/Rubrene Wedge Structure**

Manisha Priyadarsini[1], Sharanjeet Singh[1], Pooja Gupta[2,3], Ilya Sergeev[4], V. Raghavendra Reddy[1], Dileep Kumar[1a)]
[1]*UGC-DAE Consortium for Scientific Research, Indore, India*
[2]*Synchrotron Utilization Division, RRCAT, Indore-452013, India*
[3]*Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400094, India*
[4]*Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany*
[a)] *Corresponding Author's Email: dkumar@csr.res.in*

The isotope-selective grazing-incidence nuclear resonance scattering (GI-NRS) technique, a time-domain analog of Mössbauer spectroscopy, is used under X-ray standing wave (XSW) conditions to probe interface magnetism in a Rubrene/$^{57}$Fe/Rubrene trilayer. A wedge-type $^{57}$Fe layer (5–55 Å) was deposited across a single substrate, enabling thickness-dependent measurements under identical growth conditions. By tuning the incidence angle, the XSW antinodes selectively probe the top and bottom interfaces, revealing a transition from a magnetically disordered, intermixed Fe region to a well-defined ferromagnetic layer. The wedge design enables a reliable thickness-dependent study within a single sample, minimizing variability and enabling direct correlation between structure and magnetism. The results demonstrate the capability of XSW-based GI-NRS technique to resolve interface-specific magnetic behaviour in FM/OSC heterostructures.

**e0065**

**Effect of Ultrasonication Time on $TiO_2$ Termination of $SrTiO_3$ and Morphology of $SrRuO_3$ Thin Films Grown on $SrTiO_3$ Substrates**

Vinita Kumawat[1], E. P. Amaladass[1, 2], K. Ganesan[1, 2], P. Jegadeesan[1, 2], S Amrithapandian[1, 2], A. T. Sathyanarayana[1, 2] Awadhesh Mani[1, 2 *]
[1]*Condensed Matter Physics Division, Materials Science Group, Indira Gandhi Centre for Atomic Research, Kalpakkam – 603 102, India*
[2]*Homi Bhabha National Institute, Anushakthi Nagar, Mumbai, Maharashtra, India – 400 094*
*Corresponding author: edward@igcar.gov.in, vinitak@igacr.gov.in*

We investigate the effect of substrate preprocessing on the morphology of $SrRuO_3$ (SRO) thin films grown by pulsed laser deposition (PLD) on $SrTiO_3$ (STO) (001) substrates. The STO substrates were ultrasonicated in deionized water for varying durations prior to film deposition. Atomic force microscopy (AFM) confirmed that a 40-minute treatment produced a fully $TiO_2$-terminated surface. SRO thin films were then deposited using a fixed number of laser pulses across all samples. Surface morphology was characterized using both AFM and scanning electron microscopy (SEM), with the 40-minute-treated substrate enabled atomically flat, step-terraced SRO film growth. These findings highlight the importance of substrate termination quality in achieving high-quality, epitaxial oxide thin films.

**e0066**

**Thickness-dependent magnetic alignments in thin films: Investigation based on in-situ MOKE and MR measurements**

Rahul Vishvkarma[1], Ajay Gupta[2], Dileep Kumar[1,]
[1]*UGC-DAE Consortium for Scientific Research, Khandwa Road, Indore-452001, India*
*2University of Petroleum and Energy Studies, Dehradun 248007, India*
*Corresponding author: dkumar@csr.res.in*

We report an in-situ study of the thickness-dependent magnetic and magnetotransport properties of cobalt thin films grown under ultra-high vacuum conditions. Systematic in-situ Magneto-Optical Kerr Effect (MOKE) and magnetoresistance (MR)

measurements were performed along various in-plane directions of Co thin films at different thicknesses. Magnetic moment alignment across these thicknesses was investigated through MR measurements conducted in both longitudinal and transverse geometries. At approximately 50 nm thickness, anisotropic magnetoresistance (AMR) is suppressed in one of the transverse geometries, indicating an unexpected change in transverse and longitudinal MR, which we attribute to perpendicular spin alignment. Unlike MOKE—where detecting fractional perpendicular moment alignment poses challenges—MR measurements in multiple geometries provide a more sensitive method for identifying subtle variations in spin alignment along different in-plane directions. This combined experimental approach demonstrates that **in-situ** magnetotransport measurements are a powerful tool for probing moment alignment in magnetic thin films.

**e0067**

**Room temperature XPS studies of Non evaporable getter thin films**

Nidhi Gupta[1, a)], Kaushik Dutta[1,2] and Dr. Jagannath[1,2]
[1]*Technical Physics Division, Bhabha Atomic Research Center, Mumbai, 400085*
[2]*Homi Bhabha National Institute, Mumbai, 400094*
[a)] *Corresponding author: Nidhi Gupta (nidhigup@barc.gov.in)*

Non-evaporable getter (NEG) materials have emerged as a powerful solution for achieving extreme high vacuum (XHV) environments. These materials are typically deposited using sputtering techniques and are characterized using X-ray Photoelectron Spectroscopy (XPS). A variety of elemental combinations can be employed for NEG films, each offering distinct gettering properties. In this study, we have investigated a ternary combination of titanium (Ti), vanadium (V), and zirconium (Zr) as a potential NEG material. The chemical composition and surface characteristics of the films were analysed using XPS. Atomic percentage of different elements on the surface of thin film were calculated.

**e0068**

**XPS study of water adsorption on sputtered black $TiO_2$**

Mohammad Balal[1, a)] and Sudipta Roy Barman[1, b)]
[1]*UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, Madhya Pradesh, India*
*Corresponding author: [a)]mdbalal421@gmail.com, [b)]barmansr@gmail.com*

Adsorption of $D_2O$ on defect-engineered black $TiO_2$ surface has been studied using x-ray photoelectron spectroscopy at various substrate temperatures as a function of incremental $D_2O$ dosing. Thermal desorption of the $D_2O$ multilayer formed has been studied by monitoring the O 1*s* spectra as a function of temperature. On dosing, we find the presence of an undissociated $D_2O$ component and a dissociated OD component. The $D_2O$ component intensity increases with lowering temperature and increasing dosing. Interestingly, the OD component is also observed at room temperature. We observe multilayer desorption of $D_2O$ around 170 K.

**e0069**

**Bipolar Resistive Switching in Spin Coated ZrO2 thin film**

Sandeep Yadav[1], Keshav Kumar[1], Chandana Rath[1, a)]
[1]*School of Materials Science and Technology, Indian Institute of Technology (BHU), Varanasi, Uttar Pradesh, 221005, India*
a) *Corresponding author: crath.mst@itbhu.ac.in*

In this work, we report the resistive switching (RS) behavior of Zirconium dioxide (ZrO2) thin-film-based resistive random-access memory (RRAM) device deposited on Si (p++) substrate using spin coating technique with the configuration Al/ZrO2/Si. The tetragonal structure has been confirmed with X-ray diffraction (XRD) as prepared thin film. Current-Voltage (I-V) measurement shows the impressive bipolar resistive switching characteristics, including stable operation up to 250 cycles. The device exhibits low set voltage (VSet) and reset voltage (VReset), enabling reduced operating power consumption and improved energy efficiency.

**e0070**

**Observation of Spin-valve behavior in co-sputtered CoRuFeSi Heusler alloy thin films**

Shivangi Mishra[1]; Savita Sahu[2]; G.A. Basheed[2], S.N. Kaul[1] and S. Srinath[1,a)]
[1] *School of Physics, University of Hyderabad, Hyderabad-500046, Telangana, India*
[2]*CSIR-National Physical Laboratory (NPL), Dr. K. S. Krishnan Marg, New Delhi-110012, India*
[a)] *Corresponding author: srinath@uohyd.ac.in*

Spin valve (SV) devices work on the principle of controlling the resistive state by switching the magnetization of free ferromagnetic layer with respect to the pinned ferromagnetic layer. We report the SV-like behavior in 200 nm $CoRu_{0.8}FeSi_{1.2}$ (CRFS) thin films deposited at a substrate temperature of 450 ºC, 550 ºC and capped with 3nm Ta layer to prevent oxidization by oblique-angle magnetron sputtering. In addition, decrease in anti-site disorder can be seen with increase in the substrate temperature that enhances magnetic and transport properties.

**e0071**

**Anomalous Redshift and pseudo-Brewster Angle in Photonic Crystals using $TiO_2$/Ag Layered Hyperbolic Metamaterials**

Durgeshwari Rathore[1, a)], Shuvendu Jena[1, 2, b)], Dinesh V Udupa[1, 2]
[1]*Atomic & Molecular Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400 085, India*

[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai, 400 094, India*
*Email id: a) drathore@barc.gov.in; b) shujena@barc.gov.in*
The manipulation of photonic band structures in photonic crystals enables precise control over light propagation to develop advanced tunable optical devices. In this work, layered $TiO_2$/Ag hyperbolic metamaterial (HMM) is introduced in a 1D photonic crystal to explore its high anisotropy. Through combination of theoretical simulation and experimental validation, anomalous redshift of photonic band gaps and edges with increasing angle of incidence for the TM polarized light has been demonstrated in the visible region. The gaps and edges remain typically blue-shifted for the TE polarized light. Common pseudo-Brewster angles have been observed for different sets of wavelengths of TM polarized light in Type-I and Type-II HMM regions. Moreover, efficient polarization selection in a narrow band of visible region is observed in the angular range of 40°-70° making its useful for wide-angle polarization-selective photonic applications

**e0072**

**Stanene-to-Allotrope Transition in Sn Epitaxy on a Magnetic Topological Insulator**

Mrinal Manna,[1] Soumen Giri,[1] Sourav Mukherjee,[1] Pramod Bhakuni,[1] Sajal Barman,[1] Anil Gome,[1] Arnab Pariari,[2] Markus Hucker,[2] V. R. Reddy,[1] Chandana Mondal,[1] Sudipta Roy Barman,[1] Rajib Batabyal[1,*]
[1]*UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore 452001, India*
[2]*Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, Israel*
**Email: rajibbata@csr.res.in*
We investigate the structural and allotropic evolution of sequentially grown epitaxial Sn adlayers on Sb-doped MnBi2Te4 (MBST) using scanning tunneling microscopy (STM) and Grazing incidence X-ray diffraction (GIXRD) at room temperature. An initial deposition of $t_d$= 1.2 min yields a Sn–Te–Bi surface alloy (buffer layer) incorporating the topmost Te and Bi atoms of MBST with two Sn layers. Continued growth ($t_d$ = 3 min) leads to the nucleation of stanene, followed by the emergence of small 3D clusters that coarsen into multifaceted grains at higher coverages. Atomic-resolution imaging reveals a phase evolution from stanene to α-Sn in the early stages, with α- and β-Sn phases coexisting at prolonged deposition times ($t_d \geq 75$ min). GIXRD measurements validate the allotrope sequence and confirm the simultaneous presence of α- and β-Sn at later growth stages. These results establish a buffer-mediated growth pathway for Sn on MBST, governed by the interplay of lattice matching, chemical potential, and phase-transition kinetics.

**e0073**

**Magnetization Reversal and Domain Wall Dynamics in Amorphous GdCo Ferrimagnets.**

Smritiparna Ghosh [1,], Rakhul Raj[1,], Akshaya A[1,], Mukul Gupta[1,] and V. Raghavendra Reddy[1,a)]
[1]*UGC-DAE Consortium for Scientific Research, Khandwa Road, Indore – 452001, India*
**Corresponding Authors: varimalla@yahoo.com; vrreddy@csr.res.in*
The present work explores the magnetic properties and domain dynamics of amorphous GdCo alloy system. The analysis indicates that by varying the thickness and composition, we can tune the magnetic anisotropy plane and magnetic states of this alloy systems. Further, we examine the impact of varying thicknesses on domain wall dynamics.

**e0074**

**Negative Differential Resistance Assisted Resistive Switching in Chemically Grown Ca-Doped $GdMnO_3$ Thin Films**

Indrajitsinh Bihola[1], C.M. Panchasara[1], Sagar Sen[2], M. Ranjan[3], Indra Sulania[4], A.D. Joshi[5], D.D. Pandya[6], Davit Dhruv[1], P.S. Solanki[1], N.A. Shah[1], Keval Gadani[7,*]
[1] *Department of Physics, Saurashtra University, Rajkot, 360005, Gujarat, India*
[2] *Department of Physics, Maharaja Bhoj Govt. P.G. College, Dhar, 454001, India*
[3] *FCIPT, Institute for Plasma Research, Bhat, Gandhinagar 382428, India*
[4] *Inter-University Accelerator Centre (IUAC), New Delhi 110067, India*
[5] *Department of Nanoscience and Advanced Materials, Saurashtra University, Rajkot, 360005, India*
[6] *UGC: Malaviya Mission Teacher Training Centre, Saurashtra University, Rajkot, 360005, Gujarat, India*
[7] *Centre of Education, Indian Institute of Teacher Education (IITE), Gandhinagar – 382 016, India*
**Email: kjgadani@gmail.com*
We report a negative differential resistance (NDR) assisted resistive switching (RS) behavior of chemical solution deposition (CSD) grown $Gd_{0.7}Ca_{0.3}MnO_3$ (GCMO) manganite thin film on single crystalline Nb:$SrTiO_3$ (SNTO) *(100)* substrates. In order to study the structural properties, PHI - Scan measurement was performed at room temperature. To understand the RS behavior of presently studied GCMO/SNTO thin film, current–voltage (I–V) hysteresis data was taken under the sweeping bias voltages cycles: 0V → +5V → 0V → –5V → 0V across GCMO/SNTO p-n junction at room temperature. RS behavior has been discussed in terms of migration/movement of oxygen vacancies and voltage induced modification in depletion barrier across GCMO–SNTO interface. Electrical resistance of interface measured across the interface within the temperature range 150 to 300 K to determine the electrical nature of the interface. Temperature dependent I–V characteristics show the rectifying behavior having a strong thermal dependence. Interestingly, Negative Differential Resistance (NDR) behavior is observed at temperatures below 200K during forward bias, while backward diode-like characteristics emerge at temperatures below 200K under reverse bias conditions. I–V behavior has been understood with the help of Thermionic emission model.

**e0075**

**Effect of Electrostatic Interaction Between Analyte and SERS Substrate on the Coffee Ring Patterns and SERS Enhancement**

Tapan Parsain [1, a)], Sweta Gurung [2, b)], Ajay Tripathi [2, b)], Archana Tiwari [1, a)]
[1]*Banaras Hindu Univeristy, Lanka, Varanashi, India 221005*
[2]*Sikkim Univeristy,6th mile, Tadong-737102*
[a)]**Corresponding author: tparsain@bhu.ac.in*

Every Surface enhanced Raman spectroscopy (SERS) study that uses drop casted analytes on plasmonic substrates will inevitably encounter the coffee ring effect (CRE). To investigate the CRE on the performance of the SERS substrates, citrate-capped silver nanoparticles (Ag NP) were synthesized via wet chemical method. Transmission electron microscopy showed an average nanoparticle size of (37 ± 10) nm. Both anionic and cationic analytes were analyzed for trace-level identification. The surface charge of Ag NP was evaluated using Zeta potential, which is found to be – 27.5 mV at a concentration of 1.2 mg/mL and pH 7. The interaction between the analyte and nanoparticles, studied via Zeta potential analysis, revealed that oppositely charged analyte-NP mixture exhibit efficient binding compared to similarly charged mixture. In addition, particle distribution was also examined using coffee ring pattern of AgNP, the analytes and their mixtures. Subsequently the Raman mapping was performed on the mixture (with the analyte concentration $10^{-5}$ M) on the glass substrate. The distribution of oppositely charged analyte-NP mixture exhibited higher Raman scattering at the periphery of the ring whereas similarly charged mixture resulted in uniform but lower scattering in the coffee ring. The analytical enhancement factors for the detection of rhodamine 6G and methylene blue on Ag NP substrates are of the order of $10^7$ and $10^9$, with limits of detection of $10^{-7}$ M and $10^{-12}$ M, respectively. In contrast, the negatively charged analytes, such as erichrome blue T and methyl orange, show weaker enhancement with the enhancement factors $10^4$ and $10^2$ and limit of detection $10^{-7}$M and $10^{-5}$M, respectively. In order to corroborate the observed enhancement in the Raman scattering for these NPs, COMSOL Multiphysics simulation was implemented. This study on the utilization of coffee ring phenomenon for SERS substrates, offers an insight for selecting NP-analyte combinations for better signal enhancement for sensing applications.

**e0076**

**Perpendicular Magnetic Anisotropy Inflected By CoN at the Co/AlN Interface in AlN/Co/AlN Trilayer Thinfilm**

Manish [1,2], Mukul Gupta[3], P. D. Babu[4], S. D. Kaushik[4], Manvendra Kumar[5], and Parasmani Rajput[1,2*]
[1]*Beamline Development and Application Section, Bhabha Atomic Research Centre, Trombay, Mumbai-400 085, India*
[2]*Homi Bhabha National Institute, Anushakti Nagar, Mumbai-400 094, India*
[3]*UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore, Madhya Pradesh -452017, India*
[4]*UGC-DAE Consortium for Scientific Research, Mumbai Centre, R-5 Shed, Bhabha Atomic Research Centre, Mumbai 400 085, India*
[5]*Department of Physics, SVIS, Shri Vaishnav Vidyapeeth Vishwavidyalaya, Indore- 453111, India*
**Email: parasmanim80@gmail.com, parasmani@rrcat.gov.in*

We investigated the influence of CoN in the AlN/Co/AlN trilayer structure by varying the Co layer thickness. To resolve magnetic and structural properties at the Co/AlN interface, we used directional-dependent vibrating sample magnetometry (VSM) and X-ray absorption fine structure spectroscopy (XAFS). Co K-edge XAFS results revealed the quantity of CoN formation for a lower thickness of the Co sample, whereas a higher thickness of the Co sample shows pure Co hcp phase. For the lower thickness of Co, the formation of CoN shows signs of weak perpendicular magnetic anisotropy, formation at the Co/AlN interface, which is useful in spintronic devices.

**e0077**

**Effect of Mn Doping on Electrical and Optical Behaviour of Chemically Synthesized ZnTe Thin Film**

Ujjwal Prasad[1,*], Pushp Raj Harsh[1], S.R.Kumar[2], N.B.Chaure[3], K.Prasad[1]
[1]*University Department of Physics, T.M. Bhagalpur University, Bhagalpur, 812007, India*
[2]*Department of Applied Science and Humanities, NIAMT, Hatia, Ranchi,834003, India*
[3]*Department of Physics, SPPU, Pune, 411007, India*
[*)]*Email: prasadujj@gmail.com*

In this work structural properties,optical properties and electrical properties of ZnTe and Mn-doped ZnTe thin films were systematically investigated using X-ray diffraction (XRD) ,UV-Visible and current-voltage (I-V) characteristics to understand the influence of manganese (Mn) doping on the crystal structure, optical and electrical behavior of the material. Thin films of ZnTe and Mn:ZnTe were deposited using a chemical bath deposition method and characterized to evaluate their potential for optoelectronic applications, particularly in photodetectors and photovoltaic devices.

**e0079**

**Ion-Beam Engineered Temperature and Voltage Sensor with Field Tunability**

C.M. Panchasara[1], Indrajitsinh Bihola[1], Faizal Mirza[1], K. Asokan[2,3], D.D. Pandya[4], A.D. Joshi[5], Davit Dhruv[1], Keval Gadani[6], P.S. Solanki[1], N.A. Shah[1, a)]
[1]*Department of Physics, Saurashtra University, Rajkot, 360005, Gujarat, India*
[2]*Inter University Accelerator Centre, Aruna Asaf Ali Marg, New Delhi, 110067, India*

[3]*Department of Physics and Centre for Interdisciplinary Research, University of Petroleum and Energy Studies (UPES), Dehradun 248007, India*
[4]*UGC: Malaviya Mission Teacher Training Centre, Saurashtra University, Rajkot, 360005, Gujarat, India*
[5]*Department of Nanoscience and Advanced Materials, Saurashtra University, Rajkot, 360005, Gujarat, India*
[6]*Department of Physics, Center of Education, Indian Institute of Teacher Education, Gandhinagar, 382016, India*
**Email: snikesh@yahoo.com*
Temperature as well as voltage sensitivity is critical for developing, operating, and maintaining diverse electronic systems so that they operate reliably within defined parameters and needs. Manganite-based materials are extremely popular due to their properties such as Colossal Magnetoresistance (CMR), Electroresistance, Metal-Insulator transition, high sensitivity, stability, and reliability, which make them suitable for a wide range of applications such as thermoelectric devices, magnetic sensors, memory devices, spintronics, and so on. In this communication, we present the sensing capabilities of a manganite-based $Y_{0.95}Ca_{0.05}MnO_3$ (YCMO)/Nb:$SrTiO_3$ (SNTO) (100) device prepared by sophisticated Pulsed Laser Deposition (PLD) process. The films were subjected to swift heavy ion irradiation (SHI) with the 100 MeV $O^{+7}$ oxygen ions at different fluences. Structural properties were measured using an X-Ray diffractometer (XRD; θ-2θ and Φ-Scan), whereas microstructural parameters were examined with AFM. Temperature Coefficient of Resistance (TCR) of the device was measured using the Keithley manufacture 2612 A source meter coupled to a cryostat at temperatures ranging from 100K to 300K and voltages up to 2.0V to determine the device's temperature sensitivity. It demonstrated the semiconducting nature of the TCR by having a negative value, as well as improved sensing capabilities at lower temperatures, making it ideal for low temperature sensing. Along with that, the Voltage Coefficient of Resistance (VCR) values were calculated for all the pristine and irradiated films. Furthermore, it was discovered that applying an external electric field improves its detecting ability. As a result, these findings significantly support the potential of manganite-based devices for temperature and voltage sensing applications.

**e0080**
**Sequential Alkaline Etching of Ti6Al4V: A Simple Approach to Improve Surface Morphology and Bacterial Inhibition**
Sushmita Chettri [1], Deepa Seetharaman [1, (a)], Håkan Engqvist [2], Wei Xia [2, (b)]
[1] *Department of Physics, Sri Sathya Sai Institute of Higher Learning, Anantapur, Andhra Pradesh -515001, India*
[2] *Applied Materials Science, Department of Materials Science and Engineering, Uppsala University, Sweden.*
*Corresponding author: a) deepaseetharaman@sssihl.edu.in, b) Wei.Xia@angstrom.uu.se*
Titanium has been the most preferred material in the implant industry for many decades. It owes its gold standard status to its unique properties that make it one of the few biocompatible metals. However, there are several factors that need to be improved in-order to enhance the early bone to implant interaction, rapid healing, long term stability and cost efficiency. Various surface engineering strategies are implemented to address these issues. These include wet chemical etching with acids, alkalis and other agents, which is simple, cost-effective and has tremendous potential in surface engineering for better functionality.
In this study, sequential alkaline etching with NaOH followed by $NH_4OH$ was performed on Ti6Al4V at room temperature. The evolution of the surface features due to the alkali treatment and its impact on the surface morphology and surface energy were evaluated for various soaking periods ranging from 10 min to 24 h. The etched surfaces show nano-sized network formation and nearly super-hydrophilic nature. The surface with 24 h dual alkaline treatment showed higher than 70% inhibition efficiency against staphylococcus aureus.

**e0081**
**Single-atom doped 2D transition-metal dichalcogenide based SERS substrates for improved bio analyte sensing**
Nayan Guchhait[1 a)], Ankita Agrawal[1], Dileep Kumar[1], Uday Deshpande[1], Aniket Chowdhury[2], Shovan K Majumder[2,3], Arvind Yogi[1] and Debalaya Sarker[1]
[1]*UGC-DAE Consortium for Scientific Research Indore, Khandwa Road, Indore 452001, M.P, India*
[2]*Raja Ramanna Centre for Advanced Technology, Indore 452013, M.P., India*
[3]*Homi Bhaba National Institute, Department of Atomic Energy, Mumbai 400085, India*
*Corresponding Author: a) nayanguchhait0@gmail.com*
Single-atom-doped two-dimensional transition metal dichalcogenides (2D TMDCs) offer significant potential as SERS. In this work, we present a combined experimental and theoretical investigation using Rhodamine 6G as an analyte to evaluate the effectiveness of TMDC-based SERS platforms, focusing on the impact of transition metal doping. Mn was identified as a suitable dopant for enhancing the SERS activity of $MoS_2$. Both pristine and Mn-doped $MoS_2$ were synthesized via a simple chemical vapor transport (CVT) method. X-ray diffraction confirmed the phase purity of the synthesized 2D materials, while X-ray photoelectron spectroscopy and EDX validated the incorporation of Mn into the $MoS_2$ lattice and confirmed the defect-free nature of pristine $MoS_2$. Raman spectroscopy at room temperature displayed prominent $E_{2g}$ and $A_{1g}$ modes, indicating the presence of multilayer $MoS_2$. Although pristine $MoS_2$ performed reasonably well as a SERS substrate for Rhodamine 6G detection, Mn-doped $MoS_2$ demonstrated significantly enhanced SERS performance.

**e0082**
**UV Photo sensing Characteristics of $WO_3$ thin films and $WO_3$/Si Heterostructure**
Sakshi Tyagi [1], Dhruvika Tyagi[2], Shilpa Chauhan [1], Sentil Kumar Muthusamy[2*], Asokan Kandasami[1*]
[1] *School of Applied Engineering, UPES, Dehradun-248007, Uttarakhand, India.*

[2]*CSIR- National Physical Laboratory, New Delhi, India*
*Corresponding Author Email-*asokaniuac@gmail.com, senthilmk@nplindia.org*
*Author Email- sakshityagi3110@gmail.com*
With the growing demand for compact and low-power devices, environmental degradation from UV radiation exposure has become a major concern due to associated health risks like skin cancer and cataracts. In this study, tungsten oxide ($WO_3$) thin films were deposited on silicon and sapphire substrates via DC sputtering and annealed at ~600 °C for 2 hours. The glancing angle X-ray diffraction confirmed the monoclinic phase, and Rutherford backscattering analysis was used for the determination of film thickness and elemental composition. UV photodetectors were fabricated and tested under 347 nm illumination. Photo response parameters such as responsivity, detectivity, and external quantum efficiency were evaluated. $WO_3$ films on silicon exhibited the highest sensitivity with light to dark current ratio of 11.91, indicating their potential for high performance UV photodetection applications.

**e0083**

**Room temperature ammonia gas sensor based on Ti doped $Fe_2O_3$ thin films**

S. Sivaramakrishnan[1], K. Neyvasagam[1,*], S. Valanarasu[2] and V. Ganesh[3]
[1] *Research Centre and PG Department of Physics, The Madura College, Madurai – 625 011,Tamilnadu, India*
[2] *PG and Research Department of Physics, Arul Anandar College, Madurai – 625 514, Tamilnadu, India*
[3] *Central Labs, King Khalid University, P.O.Box 960, Abha, Saudi Arabia*
**Email: srineyvas@yahoo.co.in*
Ti doped $Fe_2O_3$ thin films were synthesized using nebulizer spray pyrolysis technique to study the structural, morphological and optical properties of the synthesized thin films. The XRD studies confirmed the phase purity and substitutional doping. FESEM analysis showed nanostructured particles in an agglomerated network structure with high porosity. Photoluminescence studies showed the presence of oxygen vacancies and defect states in the sample that could aid applications like gas sensors. Gas sensing studies showed a response of 1050 for 250 ppm ammonia gas with a response time of 7 s and a recovery time of 11 s for the $Fe_2O_3$ : Ti (3%) thin films.

**e0084**

**Fabrication and characterization of Ru and $B_4C$ Thin Films and Ru/$B_4C$ Multilayer via Ion Beam Sputtering**

Faiyaz Mollick[1,2*], Rajnish Dhawan[2], Jitendra Kumar[2], Ajay Kumar Kashyap[1,2], Pooja Gupta[1,2] and Maheswar Nayak[1,2]
[1]*Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai, 400094, INDIA*
[2]*Accelerator Physics and Synchrotron Utilization Division, Raja Ramanna Centre for Advanced Technology, Indore, 452013, India*
**Email: fmollick@rrcat.gov.in*
X-ray multilayer mirror plays a pivotal role in synchrotron beamlines, offering high photon flux and moderate energy resolution. Ru/$B_4C$ is one of the important material combinations for x-ray multilayer mirror for hard x-ray application. For better understanding of growth of films, the microstructural evolution with varying ion current from 20 to 90 mA at a fixed ion energy of 1000 eV of both Ru and $B_4C$ thin films deposited using ion beam sputtering (IBS) is systematically investigated. As ion current increases, film density increases as well as surface roughness decreases. At optimized parameter, the fabricated Ru/$B_4C$ ML with 10 bilayers and a periodicity of ~ 4.82 nm has an average interface roughness 0.27 nm. The density of the Ru layer in ML is smaller than the Ru thin film suggests that there may be interdiffusion of the $B_4C$ molecules into the ~ 1.95 nm thin Ru layers. This study provides insights into the understanding of effect of deposition parameters on the thin-film microstructure.

**e0085**

**Engineering Room Temperature Magneto-Optic and Ferroelectric Properties in $Co_3O_4$ Thin Films via Sb and Sm Doping Coupled with Swift Heavy Ion Irradiation Using 140 MeV $Ag^{11+}$ Ions: Structural and Defect Modulation Toward Functional Device Applications**

Jisna Rahman[1,2, a)] and Manish Chandra Joshi[3,] Chandra Sekhar M [3], Ranjith Ramadurai[3], Asokan Kandasami[4,] Rajeevan N.E[1,2]
[1]*Department of physics, Farook Autonomous College, Calicut, Kerla, 673632, India*
[2]*University of Calicut, Malappuram, Kerala, 673635, India*
[3]*Department of Material Science and Material Engineering, IIT Hyderabad, 502285, India*
[4]*Department of Physics,, University of Petroleum and Energy Studies (UPES), 248007, India*
[a)]*Corresponding author: jisnajisna@gmail.com*
This study investigates the impact of swift heavy ion (SHI) irradiation on the structural, morphological, ferroelectric and magnetic properties of $Co_{3-(x+y)}Sb_xSm_yO_{4\pm\delta}$ (x=0, 0.2 & y=0.2) synthesized by pulsed-laser ablation and irradiated with 140 MeV $Ag^{11+}$ ions. X-ray diffraction (XRD) analysis shows that SHI irradiation modulates the crystalline structure, accompanied by defect formation and track generation. Scanning electron microscopy (SEM) images reveal irradiation-induced localized densification and notable morphological changes in the films. Magneto-optic Kerr effect (MOKE) measurements indicate significant alterations in saturation magnetization and coercivity. Piezo response force microscopy (PFM) measurements demonstrate enhanced ferroelectric response and modified $d_{33}$ values, which are attributed to strain alterations due to irradiation induced tracks and defect formation. Overall, SHI irradiation provides a controllable route to tailor both structural and multifunctional properties of $Co_{3-(x+y)}Sb_xSm_yO_{4\pm\delta}$ (x=0, 0.2 & y=0.2).

**e0087**

**Influence of strain relaxation on magnetocaloric effect in FeRh thin film on MgO (001) substrate**

Rajeev Joshi[1*], Akshaya A[1], Pooja Gupta[2,3], Mukul Gupta[1] and R Rawat[1]
[1]*UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore 452001(M.P), India*
[2]*Raja Ramanna Centre for Advanced Technology (RRCAT), Indore 452013, India*
[3]*Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400094, India*
**Email: joshi.rajeev03@gmail.com*

Good quality epitaxial $Fe_{0.50}Pd_{0.47}Rh_{0.03}$ thin films on MgO (001) (30 nm and 60 nm thicknesses) were prepared by dc-magnetron co-sputtering. Structural characterization indicates high degree of Fe/Rh order in both films. However, the sign of out of plane strain turns out to be opposite for 30 nm and 60 nm thin films. Magnetization measurement shows near room temperature first order antiferromagnetic (AF) – ferromagnetic (FM) transition with relatively lower transition temperature ($T_t$) for the 60 nm film whereas remanent FM phase below $T_t$ was found to be significantly higher in the case of 30 nm film. The calculated isothermal entropy change ($\Delta S_{th}$) estimated using Maxwell relation and Clausius-Clapeyron equation are found to be in good agreement. As expected, both films show large inverse magnetocaloric effect near room temperature. Due to incomplete transformation in the case of 30 nm thin film, the peak value of $\Delta S_{th}$ is about 12 % lower than in case of 60 nm film.

**e0088**

**SCA For Searching Suitable Cutting-Edge Optoelectronic Applications in Se-Sb-Ag ACMs On Account Of LID**

Kuldeep Singh[1], Sandhya Soni[1], Shikha Shukla[1], Anjani Kumar[1*], Prince Kumar Singh[2], Rajeev Gupta[3]
[1]*Department of Physics, School of Basic Sciences, C.S.J.M. University, Kanpur- 208024, U.P., India.*
[2]*Department of Electronics and Communication Engineering, Madan Mohan Malviya University of Technology, Gorakhpur-273016, U.P., India.*
[3]*Materials Science Programme, Indian Institute of Technology Kanpur – 208002, U.P., India.*
**Email: anjanikumar51284@gmail.com*

A well-known Space charge analysis (SCA) is employed for the analysis of defect density for different illumination time, and quantitatively found Light induced defects (LID) on the thin films ($Se_{90}Sb_{10-x}Ag_x$) of Amorphous Chalcogenide Materials (ACMs) for different atomic proportions (x), which varies from 0 to 8. The outcomes show that density of defect states (DOS) raises with illumination time. The fractional increase has, however, been found to depend on the concentration of Ag in Se-Sb-Ag system. An appropriate explanation is given for LID creation in these novel ACMs and also discussed suitability for cutting-edge optoelectronic applications

**e0090**

**Effect of Annealing on Structural and Morphological Properties of $NiCo_2O_4$ Thin Films**

Kapil Kalme[1,2], Vinay Shriavstava[1], Ambrish Dwivedi[1], Salil Modak[2] Anil Gome[3,4], Yksh Gupta[5], Keval Gadani[6], Sourav Chowdhury[7] Sanjay Kumar Upadhyay[8], Mohd Rehan Ansari[9] Ratnesh Gupta[5], Sagar Sen[1,a)]
[1]*Department of Physics, Maharaja Bhoj Govt. P.G. College, Dhar, India*
[2]*School of Physics, Devi Ahilya Vishwavidyalaya, Indore, India*
[3]*UGC DAE CSR, Indore Campus, Indore, India*
[4]*Department of Physics, Medi-Caps University, Indore, India*
[5]*School of Instrumentation, Devi Ahilya Vishwavidyalaya, Indore, India*
[6]*Center of Education, Faculty of Physics, Indian Institute of Teacher Education (IITE), Gandhinagar, India*
[7]*Deutsches Elektronen-Synchrotron DESY Notkestrasse 85, 22607, Hamburg, Germany.*
[8]*HNB Garhwal University Srinagar Garhwal, Uttarakhand -246174, India*
[9]*Department of Electronic Science, University of Delhi South Campus, New Delhi, 110021, India*
*[a)] Corresponding author: sagar.sen@mp.gov.in*

$NiCo_2O_4$ (NCO) thin films were grown on Si (100) by pulsed laser deposition (PLD) and then annealed in vacuum for 1 h at 250 °C, 350 °C, and 450 °C to for 2 hours to study thermal effects. XRR showed smooth interfaces and thickness reduction from 512 Å to 465 Å, consistent with densification. GIXRD confirmed phase-pure cubic spinel with strong (400) texture, increased crystallite size, and reduced microstrain. AFM revealed surface roughness reduction from 5.15 nm to 1.63 nm with grain coarsening. Overall, vacuum annealing improves crystallinity, density, and surface quality of NCO films, making them more suitable for spintronic and energy-storage devices.

**e0091**

**Unveiling the Role of Native Oxide Formation on Si Substrate in Ellipsometric Characterization of Ion-Assisted Electron-Beam-Deposited $SiO_2$ Thin Films**

B. KaniAmuthan[1], Durgeshwari Rathore[1] R. B. Tokas[1, 2, *] and D. V. Udupa[1, 2]
[1]*Atomic and Molecular Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai*
[2]*Homi Bhabha National Institute, Mumbai*
**Email:tokas@barc.gov.in*

In this work, a $SiO_2$ thin film was deposited on a Si substrate by ion-assisted electron beam evaporation. Si was selected for its high refractive index contrast with $SiO_2$, enabling precise determination of optical constants using spectroscopic ellipsometry. Ellipsometric data (Ψ, Δ) were analyzed using both a single-layer $SiO_2$ model and a two-layer $SiO_x/SiO_2$ model. The single-layer

fit was poor (MSE ~18), whereas the two-layer model, incorporating a 4.3 nm $SiO_x$ layer, achieved an excellent fit (MSE ~3.8). The $SiO_2$ film exhibited a refractive index of 1.462 and a thickness of ~115 nm. These results demonstrate the importance of accurate optical modeling for precise characterization of thin films in high-performance multilayer optical devices.

**e0092**

**Pulsed laser deposited electron-rich micro-crystallites of MAX phases on silicon as Schottky junctions**

B.S. Revathi[1], Pramod Bankar[1], Dhanashri Sabale[2], Prachi Rajput[3], Pooja Sharma[3], S.S. Datar[1], S.N. Kale[1]*
[1]*Department of Applied Physics, Defence Institute of Advanced Technology, Pune, India*
[2]*School of Nanoscience and Biotechnology, Shivaji University, Kolhapur, India*
[3]*Central Scientific Instruments Organisation, Chandigarh, India*
**sangeetakale2004@gmail.com*

Exploring MAX and MXene materials in bulk and thin film forms has been an area of high interest, especially for miniaturised unconventional device structure, storage applications and as sensors. Considering the complex structure, achieving high-quality thin films of MAX phases is quite challenging. Of many techniques used, pulsed laser deposition (PLD) technique is one of the best routes for generating stoichiometric thin films, provided the substrates are carefully chosen. Through this work, we explore PLD of Titanium Aluminium Carbide ($Ti_3AlC_2$) MAX phase thin films on Silicon (100) substrate, focusing on film properties and possible applications. A KrF Excimer Laser (248 nm, 20 ns) was used to grow the film from MAX target. At 700°C, energy density ~2.5 J/cm², pulse repetition rate of 5 Hz, at chamber pressure of $1\times10^{-4}$ Torr, 2000 Å films were the growth on silicon substrate. Uniform, pin-hole free smooth films were seen through Electrostatic Force Microscopy (EFM). X-ray diffraction data and Raman spectroscopy data indicated stoichiometric transfer of MAX phase ((101) oriented) on the silicon substrates, however, the films were strained due to lattice mismatch (MAX phase, a =0.307 nm and silicon a =0.543 nm). There were no indications of fragmented growth. The films showed good conductivity as compared to their bulk counterparts. I-V characteristics showed excellent Schottky junction behaviour with the pick-up voltage to be 0.2 V. Conductive-Atomic Force Microscopy (C-AFM) hinted presence of free electrons on the film surface, which confirmed the metallic behaviour of the film on a semiconductor substrate. It is envisaged that stoichiometry-maintained micro-crystallites are ablated from the MAX target with laser pulses, terminating at the weakest Al-bonds; thereby generating dangling bond surfaces with large number of free electrons. The intrinsic strain facilitates this growth, which offers highly conducting film surfaces, yielding semiconductor-metal junctions. This could be explored in silicon-technology friendly non-conventional device electronics.

**e0093**

**Microstructural and Mechanical Properties of Nickel Nitride Coated NAB Prepared by Magnetron Sputtering**

Aakanksha Jain[1,2], Ramesh Chandra[2,*] and Rahul Mulik[1]
[1] *Department of Mechanical and Industrial Engineering, Indian Institute of Technology Roorkee (IIT Roorkee), Roorkee-247667, Uttarakhand, India*
[2] *Thin Film Laboratory, Institute Instrumentation Centre, Indian Institute of Technology Roorkee (IIT Roorkee), Roorkee-247667, Uttarakhand, India*
**Email:ramesh.chandra@ic.iitr.ac.in*

Nickel nitride ($Ni_3N$) thin films were fabricated on nickel aluminium bronze (NAB) substrates via DC reactive magnetron sputtering to improve mechanical performance. X-ray diffraction confirmed the formation of crystalline $Ni_3N$ with well-defined peaks, while FE-SEM images revealed a dense, uniform, and defect-free surface morphology. Energy-dispersive X-ray spectroscopy and X-ray photoelectron spectroscopy validated the elemental composition and confirmed Ni–N bonding states. The optimised deposition parameters ensured strong coating adhesion to the NAB substrate. Nanoindentation measurements recorded a hardness of 9.01 GPa, significantly higher than that of bare NAB, indicating excellent load-bearing and wear-resistant properties. These findings demonstrate that sputtered $Ni_3N$ coatings are a promising approach for extending the service life of NAB alloys in harsh industrial and marine environments

**e0094**

**Oxygen-Driven β-phase Formation in Tantalum Thin Films for Spintronics Applications**

Sonali Patajoshi[1], Madhusmita Baral[2], Vijay Kumar[3,4], and Aloke Kanjilal[1a)]*
[1]*Department of Physics, School of Natural Sciences, Shiv Nadar Institution of Eminence, Gautam Buddha Nagar, Uttar Pradesh 201314, India*
[2]*Accelerator Physics and Synchrotrons Utilization Division, Raja Ramanna Centre for Advanced Technology, Indore, Madhya Pradesh 452013, India*
[3]*Center for Informatics, School of Natural Sciences, Shiv Nadar Institution of Eminence, Gautam Buddha Nagar, Uttar Pradesh 201314, India*
[4]*Dr. Vijay Kumar Foundation, 1969 Sector 4, Gurgaon, Haryana 122001, India*
[a)] *Corresponding address of author:* aloke.kanjilal@snu.edu.in

The β-phase of tantalum (β-Ta) is highly promising for spintronic applications due to its large spin Hall angle and strong spin–orbit coupling. Yet, its formation mechanism and the role of oxygen in phase stabilization remain unexplored. In this study, we reveal how oxygen incorporation promotes the formation of the β-phase in sputtered Ta films. Detailed x-ray diffraction and microstructural analyses confirm the formation of a stable tetragonal structure, while chemical analyses show the importance of

oxygen in achieving the β-Ta phase, and our findings have been supported theoretically to understand its origin. Our results show that oxygen concentration drives phase transformation from body-centered cubic α-phase to tetragonal β-phase.

# f) Computational, AI and ML methods in condensed matter physics

**f0001**

**Structural and Electronic Properties of $Nb_3Li$**

Avinash Vyas[1,a)], Saloni Sharma[1], Vijay Maurya[2] and K.B. Joshi[1]
[1]*Department of Physics, Mohanlal Sukhadia University, Udaipur-313001, India,*
[2]*Department of Physics, Nathdwara Institute of Biotech and Management, Nathdwara-313301, India.*
a) *Corresponding author: vyasavinash2050@gmail.com*

Using the *ab-initio* FP-LAPW technique, the structural and electronic characteristics of $Nb_3Li$ are investigated. The value of vacancy migration enthalpy indicates strong interatomic bonds in the crystal. The electronic band structure reveals that similar to other A15 compounds, Niobium *d*-states contribute largely in the partial density of states.

**f0002**

**Thermal Properties of $V_3Be$**

Saloni Sharma[1,a)], Nikhil Joshi[1] and K.B. Joshi[1]
[1]*Department of Physics, Mohanlal Sukhadia University, Udaipur-313001, India.*
[a)]*corresponding author: phd22_saloni@mlsu.ac.in*

Using the ab-initio FP-LAPW method, the thermal characteristics of V3Be are investigated. The internal energy, Helmholtz free energy, entropy, heat capacity at constant volume and pressure, Grüneisen parameter, thermal expansion coefficient and Debye temperature of V3Be are determined by linking the ab-initio total energy calculations with the second-generation code Gibbs2. The calculations are performed using the Debye Slater and Debye Grüneisen models.

**f0004**

**Magnetic Properties and Critical Behavior of the J1-J2-J3 Heisenberg Model on Corner-Connected Square Units**

Pritam Manna[1] and A. K. Bera[1, 2, a)]
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India;*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*
*a)Corresponding author: akbera@barc.gov.in*

Frustrated exchange interactions in layered spin networks can stabilize a wealth of unconventional magnetic states. We investigate the classical Heisenberg model on a lattice of corner-connected square units, incorporating nearest-neighbor ($J_1$), next-nearest-neighbor within the square-units (J3), and inter-square exchange interactions (J2) by setting $|J_2|$ (inter-square interaction) as the energy scale. Constraining to inter-square ferromagnetic coupling, we map the ground-state phase diagram within $-2 \le J_1/|J_2|, J_3/|J_2| \le 2$ by combining Luttinger–Tisza minimization with extensive Monte Carlo simulations. Three distinct phases have been found: (i) a collinear antiferromagnet phase, (ii) a ferromagnetic phase, and (iii) a highly degenerate spiral phase. Large-scale Monte Carlo runs on $6 \times 6 \times 6$ supercells reproduce the Luttinger–Tisza boundaries. In addition, the thermal response of physical properties of the model like specific heat, magnetic susceptibility, staggered susceptibility, structure factors etc. have been estimated at various regions of the parameter space. This work presents a thorough investigation of the distinguished nature of temperature dependence of physical properties for all the three phases.

**f0005**

**Tunable Anomalous Hall and Nernst Effects in Magnetic Weyl Semimetals $Co_{2-x}Cr_xMnGe$**

Mainak Dey Sarkar,[1] Anumita Bose,[2,3] Arka Bandyopadhyay,[4] Dirtha Sanyal,[5,6] and Debnarayan Jana[1*]
[1]*Department of Physics, University of Calcutta, 92 A P C Road, Kolkata 700009, India*
[2]*Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560012, India*
[3]*Scuola Internazionale Superiore di Studi Avanzati (SISSA), I-34136 Trieste, Italy*
[4]*Institute for Theoretical Physics and Astrophysics, University of Wurzburg, 97074 Wurzburg, Germany*
[5]*Variable Energy Cyclotron Centre, 1/AF, Bidhannagar, Kolkata, 700064, India*
[6]*Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai, 400094, India*
**Email:djphy@caluniv.ac.in*

The discovery of magnetic Weyl semimetals has drawn significant interest due to their exceptional topological properties and anomalous transport behaviors, presenting exciting possibilities for advanced technological applications. Co-based Heusler compounds, with their unique band structures, have emerged as key materials for exploring the interplay between magnetism and topology. In this work, we perform a detailed first-principles study on Co2−xCrxMnGe Heusler alloys ($0 \le x \le 1$), proposing new candidates with significantly enhanced nontrivial transport properties. Multiple Weyl points (WPs) have been observed intrinsically in ferromagnetic Heulser alloy Co2MnGe, and the presence of bulk WPs is confirmed by the presence of isolated Fermi arcs and surface states. A significant Berry curvature is observed that arises from symmetry-protected WPs and gapped nodal lines and drives towards fascinating transport behavior. Our results show that Cr doping not only modifies the crystal symmetry but also enhances the Berry curvature, leading to a substantial effect in anomalous Hall conductivity (AHC). Notably, comparable intrinsic AHC values are observed over a range of Cr concentrations (x=0, 0.25, and 0.5) and thus demonstrate the effect of substitutional doping on topological properties as well as transport behaviours. Furthermore, we systematically explore the anomalous Nernst conductivity in these systems with Weyl fermions. These findings underscore the potential of substitutional doping to significantly enhance topological properties and anomalous transport behaviors, paving the way for the development of Co-based magnetic Weyl semimetals with superior performance in spintronic and electronic applications.

**f0006**

**Role of Vacancy Defects in Shock Compression Behaviour of Single-Crystal Tungsten: A Molecular Dynamics Study**

S. Gorai[1,2, a)], K. Basavaraj[1,2], A. S. Dwivedi[1,2], and A. Ray[1,2]
[1]*Theoretical Physics Section, Bhabha Atomic Research Centre, Mumbai, 400085*
[2]*Homi Bhabha National Institute, Mumbai, 400094*
*Corrresponding Author: *sgorai@barc.gov.in*

Extensive equilibrium molecular dynamics simulations are performed to investigate the shock response of single-crystal tungsten with presence of varying concentrations of vacancy defects, in comparison to defect-free crystals. Our study reveals a monotonic decrease in Hugoniot elastic limit with increasing vacancy concentration, showing approximately 45% reduction at 1.5% vacancies and up to 97% at 2% vacancies. Results are explained by microstructural analysis including formation of vacancies, interstitials and dislocations generated in all crystals subjected to varying shock strength encompassing elastically overdriven to plastically overdriven regimes.

**f0007**

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

P.S. Ghosh [1,2,a)] and I. Ponomareva[3]
[1]*Glass & Advanced Materials Division, Bhabha Atomic Research Centre, Mumbai 400 085, India*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai 400 094, India*
[3]*Department of Physics, University of South Florida, Tampa, Florida 66320, USA*
**Email: psghosh@barc.gov.in*

Hybrid organic-inorganic perovskites [NH2NH3][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 (DFT) 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. The DFT calculations also reveal that, under pressure, CoO6 octahedra and -HCOO ligands remain relatively rigid while CoO6 octahedra tilt significantly, which leads to highly anisotropic mechanical properties and expansion along certain directions.

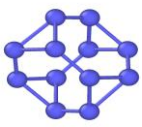
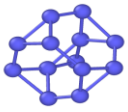
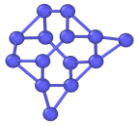
**f008**

**Determination of Transition Energies of C15-like Defect Clusters in Tungsten using Molecular Dynamics**

D. Charitha Durga[1], P.V. Lakshmi Narayana[1], S. Choudhary[2], U. Bharadwaj[3], M.Warrier [3,4]
[1] *Department of Nuclear Physics, Andhra university*
[2] *Institute for Plasma Research, BHAT, Gandhinagar, Gujarat, India*
[3] *Computational Analysis Division, BARC Visakhapatnam,*
[4] *Homi Bhabha National Institute, Mumbai*
*Corresponding Author *doddicharithadurga735@gmail.com*

Irradiation of tungsten by neutrons or high energy ions creates energetic primary knock-on atoms (PKA) in the material. These energetic PKA creates local collision cascades of a few picoseconds duration. Initially a large number of lattice atoms are displaced which subsequently recombine to form the primary damage consisting of self interstitial atoms (SIA), vacancies and clusters of these defects. These defect clusters in tungsten have been classified into six different classes as described by Bharadwaj et al., [1]. The evolution of the primary damage depends on the stability of these defect clusters. One of the classes of defect clusters is the C15 defect cluster. We have studied the stability of 11 different C15 clusters (see figure-1) by carrying out 24 different molecular dynamics simulations for each cluster for statistics. A crystal with the isolated C15 cluster is subjected to a temperature ramp from 300k to 2100k for a duration of 100 nanoseconds. From the simulations, we have extracted the average transition times and the average transition temperatures. We assume an Arrhenius like transition and calculate the transition energies and their associated errors for each cluster. The transition energies of the clusters lie between 0.4±0.3 eV – 1.91±0.3 eV.

Keywords: Collision Cascades, Molecular Dynamics, Defect Cluster, tungsten, ramp, Transition energies.

| 2-C | 3-C | 3-Tripod | 4-C |
|---|---|---|---|
|  |  |  |  |

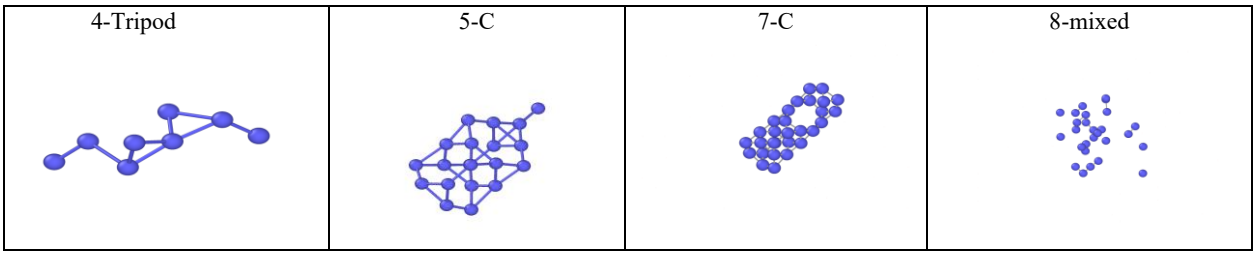



FIGURE 1. The figure shows the representative relaxed structures for eight distinct C15 like cluster types: 2C, 3C, 3Tripod, 4C, 4Tripod, 5C, 7C, and 8mixed. The numerals before each "C" indicates the number of interstitials in the cluster. These configurations were extracted the primary damage resulting from MD simulations of collision cascades in tungsten and their transition energies are studied in this paper using MD simulations.

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U. Bhardwaj, A. E. Sand, M. Warrier, Graph theory based approach to characterize self interstitial defect morphology, computational Material Science 195 (2021) 110474.

**f0010**

**Topological Phase Transition of $TiS_3$ under Pressure**

A R Atique Ulla[1,2,*] and P. Modak[1,2]

[1]*High pressure and Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, India*

[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*

**Email: atiqueulla@gmail.com*

At ambient pressure, $TiS_3$ crystallizes in a centrosymmetric monoclinic structure (space group P21/m) with quasi-one-dimensional trigonal prismatic chains. Density functional theory calculations show it is a topologically trivial insulator with a direct band gap and no band inversion. Under hydrostatic pressure, the band gap closes and reopens with a reversal in orbital character, indicating a topological phase transition. Z2 invariant analysis confirms a transition to a strong topological insulator phase with (1; 111) indices. Surface state calculations reveal robust, gapless Dirac states with spin-momentum locking. These results highlight TiS3 as a potential candidate for studies of pressure-driven topological quantum phases.

**f0011**

**First-principles calculations on Cr doped $Bi_2Se_3$ topological insulator**

Ravi Kumar[*, 1, 2] and Dibyendu Bhattacharyya[1, 2]

[1]*Atomic & Molecular Physics Division, Bhabha Atomic Research Centre, Mumbai-400 085, India*

[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai- 400 094, India*

**Email: raoravi@barc.gov.in*

Magnetic ion doping in topological insulators has gained significant attention, both for its technological relevance and for probing exotic fundamental physical phenomena. A comprehensive understanding of the atomic configuration and electronic state of magnetic dopants within the topological insulator lattice is crucial for unraveling the physical behavior of these systems. In this work, we have systematically investigated the impact of Cr doping on the structural and electronic properties of $Bi_2Se$. First-principles calculations based on Density Functional Theory were performed, considering Cr atoms substituted at Bi sites as well as at various interstitial positions. We have evaluated the formation energies, electronic structures, and magnetic properties of Cr-doped $Bi_2Se_3$. Additionally, we have simulated the influence of Cr doping on the topological surface states to understand its effect on Dirac cone characteristics.

**f0012**

**Development and Experimental Validation of a FLUKA-Based Monte Carlo Model for a Portable HPGe Detector**

Pratip Mitra[1, a)], Amar Dutt Pant[1], Amit Kumar Verma[1], R. S. Sathyapriya[1] and S. Anilkumar[1]

[1]*Environmental Monitoring and Assessment Division, Bhabha Atomic Research Centre, Mumbai 400085, India*

**Email: pratipm@barc.gov.in*

This study presents the development and experimental validation of a detailed FLUKA-based Monte Carlo model of the Canberra GC2018 portable high-purity germanium (HPGe) detector. The detector was modeled using manufacturer supplied dimensions. Energy calibration and full width at half maximum (*FWHM*) measurements were performed using standard gamma-emitting radionuclides including $^{133}Ba$, $^{137}Cs$, and $^{60}Co$. The experimentally obtained FWHM values were fitted as a function of energy and used to apply Gaussian broadening to the simulated spectra. The simulated $^{60}Co$ spectrum generated with a source-to-detector distance of 25 cm was compared with the measured spectrum. Relative efficiency values from both experiment and simulation were also compared, and were in good agreement. The validated FLUKA detector model enables reliable efficiency calibration for practical geometries and supports virtual calibration in field applications where experimental calibration is not feasible.

**f0013**

**Primary Damage in Niobium: Comparing a ML based Potential with Classical Potentials**

Suman Mondal[1,a)], U. Bhardwaj[1], A. Majalee[1], V. Mishra[1,2], M.Warrier[1,2]
[1] *Computational Analysis Division, BARC Visakhapatnam,*
[2] *Homi Bhabha National Institute, Mumbai*
*asmondal@barc.gov.in*
Primary radiation damage in bcc niobium was examined using molecular dynamics (MD) simulations of collision cascades for PKA energies ranging from 1 to 75 keV with three classical interatomic potentials: EAM, FS-1, FS-2, and a machine Learning (ML) based potential: SNAP. The ML potential was developed in-house by fitting several hundreds of DFT simulation results for various configurations of niobium atoms. 25 PKAs were launched in random directions at each PKA energy for statistics. While all the potentials capture general trends, they differ in the kind of primary damage produced, specifically the damage morphology. The EAM potential consistently results in the highest peak and surviving defect counts, strong vacancy clustering, and is also the only potential to occasionally predict rare ⟨100⟩ dislocation loops at high PKA energies. FS-2 shows dominant formation of extended 1/2⟨111⟩ dislocation loops, which are observed in bcc metals. FS-1 and SNAP tend to form compact or disordered clusters and C15 like rings, with SNAP exhibiting the highest interstitial clustering. The ring formation may be attributed to the FS1 and SNAP potentials being trained on amorphous / liquid configurations.

**f0014**

**Quantum Spin-Hall Insulators in Square-Octagonal $MSi_2Z_4$ (M = Transition Metal, Z = Pnictogen)**

Rahul Verma[1,*] and Bahadur Singh[1]
[1]*Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Mumbai 400005, India*
**Email: rahul.verma@tifr.res.in*
Two-dimensional quantum spin Hall (QSH) insulators protected by time-reversal symmetry exhibit counter-propagating spin-polarized helical edge states and are promising candidates for spintronic devices. However, their spin Hall conductivity is often not quantized due to the breaking of spin U(1) symmetry by spin mixing induced by strong spin-orbit coupling. In this work, we predict a new class of QSH insulators in the seven-layered $MSi_2Z_4$ family, which realize large-gap QSH insulators in their square-octagonal polymorphs. Spin-resolved topology and symmetry analysis show that these systems support a spin Chern number $C_s$=1 and host $S_z$ spin-polarized edge states. The QSH phase exhibits an emergent spin U(1) quasi-symmetry, leading to nearly quantized spin Hall conductivity of $2e^2/h$. Among these materials, $WSi_2Sb_4$ displays flat-band-like dispersions and higher-order van Hove singularities near the Fermi level, offering a platform for exploring correlated QSH phases.

**f0015**

**Characterization of Organic Co-Crystal by Powder X-ray Diffraction and Vibrational Spectroscopy with DFT Computation**

[1]Sameer Kumar Singh, [2]Mohd Faizan, [3]Md. Masroor Ahmed
[1] *P.G. Department of Physics, Magadh University Bodh-Gaya, Bihar-824234*
[2,3] *Mirza Ghalib College, Gaya (Magadh University Bodh-Gaya, Bihar-823001*
**Email: mausamkumar084@gmail.com*
This work mainly focused on the crystal structure, vibrational spectral studies of the grown cocrystal between 2,3-dimethylquinoxaline (DMQ) and 3,5-dinitrobenzoic acid (DNB) molecules. The combined powder X-ray diffraction (PXRD) and Rietveld refinement analysis have been utilized to investigate the nature of crystal structures and affirm phase purity of the co-crystal. The cell parameters suggest that the co-crystal belongs to an orthorhombic structure. The vibrational spectral properties of the complex molecule have been studied using FTIR and simulated spectral analysis. The anharmonic corrections in vibrational wavenumbers are carried out using the GVPT2 method at B3LYP/6-311G(d,p) level of theory. Furthermore, the density functional theory (DFT) method is successfully applied to calculate natural atomic charges.

**f0016**

**First-Principles Investigations of Structural and Electronic Properties of Lead-Free Double-Perovskite Halide $Cs_2AgBiBr_6$ Using WIEN2K**

Monika Sharma[1,*], Jatin Sharma[1], Ashok Kumar Sharma[2] and Vikas Thakur[3]
[1]*Sardar Patel University, Mandi, Himachal Pradesh-175001, India*
[2]*Madhav Institute Of Technology & Science, Gwalior (M.P.) -474005, India*
[3]*Govt. Degree College Bassa (Gohar), Mandi, Himachal Pradesh-175029, India*
[*]*Email: monikasharma@spumandi.ac.in*
In recent years, double perovskite materials have been considered potential candidates for different applications. Therefore, in this study, we investigated the structural and electronic properties of $Cs_2AgBiBr_6$ – a lead free double perovskite halide based on first-principles calculations using the WIEN2K computational package within the framework of DFT. The material was structurally optimized and the lattice constant was determined. The electronic band gap and DOS reveal that $Cs_2AgBiBr_6$ is an indirect band gap semiconductor. Our analysis demonstrates that $Cs_2AgBiBr_6$ is a suitable material for photovoltaic and optoelectronics applications.

**f0017**

**Achieving High Efficiency of 28.85% in $Cs_4CuSb_2Cl_{12}$-Based Perovskite Solar Cell Using SCAPS Simulation** Shramank Chaturvedi and Arpana Agrawal[a)]

*Department of Physics, Prime Minister College of Excellence, Shri Neelkantheshwar Government Post-Graduate College, Khandwa-450001, India.*

*[a)] Corresponding author: agrawal.arpana01@gmail.com*

Significant efforts have been devoted to improving the performance of solar cells, with perovskite-based materials gaining attention due to their outstanding optoelectronic properties. In the present work, the photovoltaic performance of a lead-free $TiO_2/MoS_2/Cs_4CuSb_2Cl_{12}/Cu_2O$ perovskite solar cell (PSC) structure has been investigated using SCAPS-1D simulation. The Cu-Sb halide perovskite offers enhanced environmental stability and lower toxicity compared to conventional lead- and tin-based alternatives. Key device parameters, including short-circuit current density ($J_{SC}$), open-circuit voltage ($V_{OC}$), fill factor (FF), and power conversion efficiency (PCE), were analyzed to assess performance. The influence of absorber layer thickness and $MoS_2$ electron transport layer thickness on cell efficiency was systematically studied. Optimization of the absorber thickness from 100 to 1000 nm led to a 4% increase in efficiency, with a peak PCE of 21.25% at 600 nm. Further tuning the ETL thickness to 500 nm resulted in a maximum PCE of 28.85%. These results highlight the potential of Cu-Sb perovskites and $MoS_2$ as promising, for high-efficiency, stable solar cells.

**f0018**

**A Holistic Exploration of Structural, Elasto-Mechanical and Electronic Properties Cobalt Based Quaternary Heusler Alloy CoCrTiSb**

Shashank Nautiyal* and Meena Kumari

**Department of Science, Mewar Institute of Management, Sector 4C, Vasundhra Ghaziabad, U.P. India-201012*

*Department of Physics, Himachal Pradesh Technical University, Hamirpur, H.P. India*

**Email:shashank.fiziks.ju93@gmail.com*

First principles study of structural, elasto-mechanical and electronic properties of cobalt based quaternary Heusler alloy CoCrTiSb have been reported in this article. All the calculations have been performed within the framework of density functional theory based full potential linearized plane wave method as implemented in Wien2k package. Structural parameters are obtained by performing structural optimization. Obtained elastic parameters shows that given compound is ductile and anisotropic in nature. Electronic band structure plot indicates that CoCrTiSb is semiconducting in nature which is also confirmed from density of states plot.

**f0019**

**A Thorough Investigation Of The Optoelectronic Properties Of $Rb_2YAuX_6$ (X= F, Cl, Br, I) For Solar Cell Applications**

Angela Chinggelkim[1,2] and Lalhriat Zuala[2,*]

*[1]Department of Physics, Mizoram University, Aizawl 796004, India*

*[2]Physical Sciences Research Center (PSRC), Department of Physics, Pachhunga University College, Mizoram University, Aizawl 796001, India*

*[*]Corresponding author: hriata@pucollege.edu.in*

Although double halide perovskites have garnered significant attention as environmentally benign and structurally versatile alternatives to lead-based counterparts, the optoelectronic behavior of the $Rb_2YAuX_6$ (X= F, Cl, Br, I) remain underexplored. Given the favorable band gaps 1.47, 2.04, 1.63 and 1.13 eV (GGA) and 1.19, 1.85, 1.48 and 0.94 eV (GGA+SOC) and stability often associated with gold-based perovskites, and the significant impact of spin-orbit coupling due to the presence of heavy elements like gold, theoretical calculations were performed using Density Functional Theory on the double halide perovskite compound $Rb_2YAuX_6$ (X= F, Cl, Br, I). We have found that the computed band gaps and the most active optical absorption are within the Vis-UV range with an absorption coefficient $\alpha > 10^5$ $cm^{-1}$, suggesting that these materials are highly promising for the development of efficient and stable light-harvesting materials for next-generation solar energy technologies.

**f0020**

**The Structural, Mechanical and Electronic Properties of Non-centrosymmetric $Sc_6MTe_2$ (M = Fe &Os) compounds**

N.K. Sarkar[1], P.S. Ghosh[2,3], K. Ali[2]

*[1]Materials Science Division, Bhabha Atomic Research Center, Trombay, Mumbai, India*

*[2]Glass & Advanced Materials Division, Bhabha Atomic Research Center, Trombay, Mumbai, India,*

*[3]Homi Bhabha National Institute, Mumbai-400094, India*

**Email: nilabja@barc.gov.in (Email of corresponding author)*

First-principles DFT calculations have been employed to investigate the structural, mechanical and electronic properties of ternary Sc6MTe2 (M = Fe and Os,) compounds. The optimized crystal parameters show good agreement with the available experimental and theoretical data. The mechanical properties, including the independent elastic constants, bulk modulus, shear modulus, Young's modulus, pugh ratio (B/G), Poisson's ratio along with anisotropy constants have been systematically estimated. The electronic structure, analyzed via band structure and density of states, reveals metallic behavior with characteristic features relevant to non-centrosymmetric systems.

**f0021**

**First Principles Study of Strain Induced Modulation of Electronic Properties in $Cu_2Se$**

Hashir P[1,*] Hridya B Krishna[1] P P Pradyumnan[1]
[1]*Department of Physics, University of Calicut, Malappuram-673635, Kerala, India*
**Email:hashirp.916@gmail.com*
In this DFT study, the strain-dependent electronic properties of cubic $Cu_2Se$, a narrow band gap p-type semiconductor, were investigated using Quantum Espresso software within the Generalized Gradient Approximation combined with Hubbard U correction (GGA+U). Isotropic strain ranging from −4% (compressive) to +4% (tensile) was applied to assess its impact on the electronic band structure. The results reveal a clear correlation between applied strain and band gap modulation, with the valence band maximum and conduction band minimum showing high sensitivity to lattice deformation. These changes are attributed to alterations in orbital hybridization and band dispersion, highlighting strain engineering as an effective approach to tune the electronic properties of $Cu_2Se$.

**f0022**

**Ionic Diffusion in $Na_3OCl$ Solid Electrolytes: An Atomistic View from Machine Learned Molecular Dynamics**

Samiran Malgope[1,2], Mayanak Kr. Gupta[1,2, a)], Prabhatasree Goel[1,2], Ranjan Mittal[1,2], Samrath Lal Chaplot[1,2]
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai, 400085, India*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*
**Email: mayankg@barc.gov.in (Email of corresponding author)*
Antiperovskites show promise as high-performing Li/Na electrolytes due to their tunable structure, high ionic conductivity, and stability against dendrite formation. $Na_3OCl$ is a promising antiperovskite Na-solid electrolyte due to its robust sodium-ion conductivity and favourable structural characteristics. In this work, we present a comprehensive molecular dynamics investigation of $Na^+$ diffusion in $Na_3OCl$. Our large-scale machine learned molecular dynamics simulations reveal pronounced three-dimensional diffusion pathways, with an estimated diffusion coefficient of $3.5 \times 10^{-7}$ $cm^2/s$ at 900 K and an activation energy around 0.55 eV, closely matching recent experimental reports. Our study reveals that sodium vacancies are the primary facilitators of ion migration, while a few key phonons further accelerate these processes, enabling fast $Na^+$ diffusion in Na3OCl. The atomistic insights provided here reinforce the potential of $Na_3OCl$ antiperovskite as a next-generation solid electrolyte and offer valuable guidelines for the rational design and optimization of solid-state sodium-ion batteries

**f0025**

**Enhancing Detection Sensitivity of Infrared Spectra of Molecular Mixtures with Artificial Intelligence Modeling**

Debjani Bagchi[1, *,] Manali Pancholi[1], Rohan Kumar Sethy[2], S. S. Roy[1], and Aayushi Raval[1]
[1]*Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat 390002, India.*
[2]*Department of Physics and Astronomy, National Institute of Technology, Rourkela, Odisha, India, 769008.*
**Email:debjani.bagchi-phy@msubaroda.ac.in (Email of corresponding author)*
A wide array of spectroscopic tools can presently enable detection of molecules present in extra-terrestrial systems, or environmental pollutants such as microplastics, diagnostic and clinical practices, energy and geophysical research. This entails the development of faster detectors with high quantum efficiency to improve sensitivity of molecular detection with spectroscopic techniques. The very next step of detection is spectral analysis, and algorithms helping molecular spectral modeling are imperative for identification of molecular species. To this end, machine learning algorithms have enabled efficient classification tools. Using different classification tools, we have tried to identify the major components of agricultural wastes for easing bioenergy production from these systems. In case of agricultural waste, the template matching algorithm is used to detect the presence of cellulose within lignocellulose, thereby analyzing the applicability of the agricultural waste for bioenergy applications. Moreover, modeling the agricultural waste spectral data with neural network algorithms show reasonably good accuracy between the predicted and the experimental values. We also explore some pattern recognition algorithms such as spectral de-mixing and non-negative matrix factorization to detect simple astromolecules in binary and ternary mixtures.

**f0026**

***Ab-initio* Investigation of *h*-$Be_3N_2$ Monolayer for Photocatalytic Hydrogen Evolution Reaction**

Karan Patel, Hetvi Jadav, Himanshu Pandey*
*Condensed Matter & Low-Dimensional Systems Laboratory, Department of Physics, Sardar Vallabhbhai National Institute of Technology Surat-395007, Gujarat, India*
*Corresponding author: hp@phy.svnit.ac.in*
The demand for a sustainable, renewable, and eco-friendly energy source is increasing due to the continuous consumption of fossil fuels. Recently, the research trend has gained significant attention among researchers on photocatalytic hydrogen evolution reaction (HER) due to limited hydrogen evolution efficiency. In this work, we perform a first-principles study on a 2D *h*-$Be_3N_2$ monolayer using density functional theory to investigate its structural, electronic, and catalytic properties. The result obtained from the band structure indicates that $Be_3N_2$ exhibits a direct bandgap semiconductor. Furthermore, the Gibb's free energy and favorable band edge positions aligned with the redox potentials of water, making it a suitable candidate for visible-light-driven photocatalysis for HER.

**f0027**

**Computational Design of Si-doped-LiPON Solid Electrolyte for All-Solid-State Lithium-Ion Battery**

Archana Hota[1], Siddharth Sradhasagar[1] and Amritendu Roy[1*]
[1]*Functional Materials Laboratory, School of Minerals, Metallurgical and Materials Engineering, Indian Institute of Technology Bhubaneswar, Khordha, Odisha, India*
**amritendu@iitbbs.ac.in (Email of corresponding author)*
This study investigates the potential of silicon (Si) doping in $Li_{14}P_2O_3N_6$ (LiPON) solid electrolyte to enhance its electrochemical and ionic transport properties for all-solid-state lithium-ion battery applications. Using first-principles Density Functional Theory (DFT) calculations, the structure of Si-doped LiPON (LiPSiON) was optimized to identify the most stable configuration and assess its structural stability. Electronic properties were analyzed through band structure and density of states (DOS) calculations. Additionally, room-temperature diffusivity and ionic conductivity were quantitatively predicted using *ab initio* molecular dynamics (AIMD) simulations, confirming the potential of Si-doped LiPON as an advanced solid electrolyte. This work offers valuable insights for the computational design of next-generation energy storage materials.

**f0028**

**Investigating Optical Isotropy in Structurally Anisotropic Halide Double Perovskites $X_2MgCl_4$ (X = Na, K, Rb, and Cs)**

Phamei Rumthao[1] and G. Vaitheeswaran[1,*]
[1]*School of Physics, University of Hyderabad, Prof. C. R. Rao Road, Gachibowli, Hyderabad, 500046, Telangana, India*
**Email: vaithee@uohyd.ac.in (G. Vaitheeswaran).*
We investigate the structural, electronic, and optical properties of a series of halide double perovskites, $X_2MgCl_4$ (X = Na, K, Rb, Cs), using first-principles density functional theory calculations. These materials crystallize in an orthorhombic layered structure and demonstrate remarkable thermal and chemical stability. Despite their intrinsic structural anisotropy, our optical analyses reveal a surprising degree of isotropy in the dielectric response. The band structure calculations indicate wide band gaps in the range of 6.37–6.46 eV, with $Cs_2MgCl_4$ exhibiting the maximum gap. Charge density distribution confirms the ionic nature of bonding, and core–valence excitations suggest favorable conditions for radiative recombination. The optical isotropy, in conjunction with the feasibility of growing large single crystals, highlights the potential of $X_2MgCl_4$ compounds for advanced scintillation and optoelectronic applications.

**f0030**

**Lattice Dynamics Calculations Of $Li_3TiCl_6$**

Anuradha Sharma[1, a)], and Mala N. Rao[1, 2]
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India.*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India.*
[a)] Corresponding author: asharma@barc.gov.in
Lattice dynamics calculations have been carried out for $Li_3TiCl_6$. Phonon dispersion curve, phonon density of states are computed. Using phonon density of states we have computed variation of specific heat with temperature.

**f0033**

**Inverse Design of 1D Photonic Crystal Reflectors Using a Physics-Informed Genetic Algorithm for Broadband Mid-IR Gas Sensing**

Abhishek Bhardwaj, Danish Kumar, Sandeep Sharma and K. K. Sharma
*Department of Physics and Photonics Science, National Institute of Technology Hamirpur, (H.P.)-177005, INDIA*
**Email: abhishek.academia@gmail.com*
This paper presents a physics-informed inverse design methodology for optimizing one-dimensional photonic crystal structures to achieve wideband reflectors tailored for mid-infrared gas sensing applications. A genetic algorithm, integrated with a Transfer Matrix Method-based spectral simulator, is employed to inversely determine the optimal layer thicknesses ($d_1$, $d_2$) and number of bilayer periods (N) required to achieve user-defined stopbands with zero edge error and ultra-high reflectivity (>99.9%). For a target stopband of 600 nm (2900–3500 nm), the proposed design achieves a total thickness of just 4.166 μm. Compared to conventional quarter-wavelength stack designs, which are constrained by their central wavelength and require significantly greater thickness to cover broadband ranges, our approach achieves the user specified performance with a ~6% reduction in total thickness. This compact and customizable reflector design facilitates the development of integrated and miniaturized gas sensing systems.

**f0035**

**A Machine Learning and Molecular Dynamics Based Method to Predict the Temperature Dependent Young's Modulus of Silver Nanowires**

Riya Gola[1], Harendra Singh Bohara[2], Mahipal Singh[1] and S. K. Joshi[3,*]
[1]*Department of Physics, R.H. Govt. P.G. College, Kumaun University, Nainital-263001, India*
[2]*Department of Applied Sciences, Birla Institute of Applied Sciences, Bhimtal-263136, India*
[3]*Department of Applied Sciences, Shivalik College of Engineering, Dehradun- 248007, India*
**mail.skj@gmail.com*
Studying the mechanical characteristics of nanowires is essential to enhance their efficient utilization in a variety of nanoscale devices. In the present investigation, firstly we have performed MD simulations using LAMMPS to study stress-strain behavior

and young's modulus of silver nanowires at different temperatures. Then we train and evaluate several machine learning models, such as Linear Regression, Support Vector Machine (SVM), Gaussian Process Regression (GPR), Neural Networks (NN), Fine trees and Ensemble Bagged Trees algorithms to predict the young's modulus by utilizing a dataset obtained from MD Simulations of Ag NWs at various temperatures. We evaluated the performance of the models using standard regression metrics such as Root Mean Squared Error (RMSE), R-Squared Value ($R^2$), Mean Squared Error (MSE), Mean Absolute Error (MAE). Results from this study show that the GPR model provides the highest predictive accuracy, closely followed by the LR, SVM and NN, while the Fine Trees and Ensemble bagged trees regression model demonstrated lower predictive accuracy.

**f0037**

**Electronic And Thermoelectric Investigation Of CoZrAs Heusler Alloy Using Ab-initio Formulism**

Sadhana Matth[a], Himanshu Pandey[a*]
*Condensed Matter & Low-Dimensional Systems Laboratory, Department of Physics, Sardar Vallabhbhai National Institute of Technology Surat-395007, Gujarat, India*
*Corresponding author: hp@phy.svnit.ac.in*

In this study, the electronic and thermoelectric properties of cobalt-based *half*-Heusler alloy are investigated through first-principles calculations by employing the Quantum Espresso package. Initially, the crystal structure was optimized to obtain the ground state and thus to estimate the lattice parameter and structural properties. Using these optimized parameters, the band structure for the CoZrAs alloy was analyzed, revealing an indirect band gap of approximately 1.26 eV in the spin-up channel. The maximum power factor (*PF*) observed was approximately $1.39\times10^{12}$ $Wm^{-1}K^{-2}s^{-1}$ at a temperature of 850 K. Our computed dimensionless figure of merit at is 3.21 at 850K; this represents that our alloy could be a better material for thermoelectric applications.

**f0038**

**Structural, Electronic And Magnetic Properties Of Ni Nanoalloy : A Combined First Principle And Experimental Study**

Aiswarjya Bastia[1] and Chandana Rath[1*]
*[1]School of Materials Science and Technology, Indian Institute of Technology (BHU), Varanasi, Uttar Pradesh, 221005, India*
*[*]Corresponding author: crath.mst@itbhu.ac.in*

The present work investigates a first-principle density functional theory (DFT) calculation on the structural, electronic, and magnetic properties of Ni nanoalloy. Using the generalized gradient approximation (GGA) within the Perdew–Burke–Ernzerhof (PBE) framework, we analyze band structure, density of states (DOS), and magnetic moment. By minimizing the total energy, structural optimization yields a lattice constant and unit cell volume that closely match experimental observations. Magnetic calculations illustrate a ferromagnetic ground state with the total magnetic moment per formula unit aligning well with previously reported moment. Further analysis with electronic band structure and DOS shows the metallic nature and overlapping of spin-split bands at $E_F$. The observed asymmetry between the spin-up and spin-down states, is ascribed to the strong hybridization of Ni 3d orbitals. Overall, these findings confirm that the PBE-GGA approach is indeed reliable for computational analysis of Ni and other transition metal nanoalloys in regard to their electronic and magnetic characteristics.

**f0039**

**Tunable Electronic Properties of MXene/blue Phosphorene Heterostructures under an External Electric Field**

Sarga P K and Swastibrata Bhattacharyya *
*Department of Physics, Birla Institute of Technology and Science, Pilani, K K Birla Goa Campus, Zuarinagar, Sancoale, Goa 403726, India.*
** Corresponding author: swastibratab@goa.bits-pilani.ac.in*

Van der Waals (vdW) heterostructures based on two-dimensional (2D) materials offer exciting opportunities by combining the strengths of individual layers. Of particular interest is the type-I to type-II band alignment transition, which enhances charge separation for photocatalytic and optoelectronic applications. Using *ab initio* calculations, we investigate the electronic properties of the MXene ($Sc_2CO_2$, $Zr_2CO_2$, and $Hf_2CO_2$) /blue phosphorene heterostructures. A perpendicular electric field is applied to tune its electronic properties, leading to notable changes in band gap and alignment without affecting structural integrity. These results highlight MXene/blueP heterostructures as promising candidates for tunable nanoelectronic and optoelectronic devices.

**f0040**

**First-Principles Insights into Structural, Electronic and Optical Properties of Janus β-$TiPb_2N_4$**

Rohit Kumar[1, a)], Ankush Bharti[1,2] and Raman Sharma[1]
*[1]Department of Physics, Himachal Pradesh University, Summer-Hill, Shimla 171005, India*
*[2]Rajiv Gandhi Government Polytechnic, Banikhet, Chamba (Himachal Pradesh) 176303, India*
*Email: rohit35700885@gmail.com*

We propose a novel two-dimensional (2D) Janus semiconductor $\beta - TiPb_2N_4$ and investigate its properties using first-principles DFT calculations. The material is a direct-gap semiconductor with a band gap $E_g = 0.94eV$. Calculated formation energy is negative, indicating energetic stability. Phonon and AIMD simulations at 300 K for 5 ps show no imaginary modes or structural degradation. The absorption spectrum exhibits peaks at 4.14 eV ($\omega \approx 1.0 \times 10^{15}s^{-1}$). and 6.18 eV ($\omega \approx 1.5 \times 10^{15}s^{-1}$).

Reflectance remains very low (3%) across the studied range. These results suggest $\beta - TiPb_2N_4$ is a dynamically and mechanically robust 2D semiconductor with strong ultraviolet absorption, promising for optoelectronic applications.

**f0042**

**Structural And Electronic Properties Of LaSn3-xGex (x = 0, 1, 2, 3) Compounds: DFT Calculation**

Hansa Devi[1,a)] Jyotsana Sharma[1]
[1]*Department of Physics, Swami Vivekanand Govt. College Ghumarwin, Himachal Pradesh University, Shimla-175027, India*
[a)]*Corresponding author: hansa.phy@gmail.com*

The structural and electronic properties of non-magnetic $LaSn_{3-x}Ge_x$ (x= 0, 1, 2, 3) have been systematically investigated within the framework of density functional theory (DFT). Structural stability and volume change due to the addition of Ge, on $LaSn_{3-x}Ge_x$ (X = 0, 1, 2, 3) have been computed by applying full-potential linearized augmented plane wave (FP-LAPW) method. The equilibrium structural parameters for $LaSn_3$, $LaSn_2Ge$, $LaSnGe_2$ and $LaGe_3$ compounds are calculated and compared with the available experimental as well as theoretical data. The computed band structures reveal that the doping of Ge does not change the metallic nature of $LaSn_2Ge$, $LaSnGe_2$ and $LaGe_3$.The calculated density of states at Fermi level $N(E_F)$ shows that all these compounds are metallic in nature and $LaGe_3$ is found to be the most metallic.

**f0043**

**Bayesian Implications for Theoretical Bandgap Prediction**

Ashish Sharma[1, a)], Vivekanand Shukla[1], and Raj Kumar[2]
[1]*Computational Materials Physics Laboratory, Department of Physics, Indian Institute of Technology Ropar, Rupnagar 140001, Punjab, India*
[2] *Computational Astrophysics Group, Department of Physics, Himachal Pradesh University Shimla, SummerHill, 171005, H.P., India*
[a)]Corresponding author: ashishsharma.physics@gmail.com

Density functional theory (DFT) is an essential computational tool for predicting electronic properties of materials but is well known to systematically underestimate bandgaps, limiting its direct quantitative agreement with experiments. In this work, we present a Bayesian calibration workflow that explicitly models and corrects for this systematic error by combining DFT calculated bandgaps with available experimental reference data. Using a hierarchical Bayesian framework and robust Markov Chain Monte Carlo (MCMC) inference, we jointly estimate the systematic offset and intrinsic noise in DFT predictions, yielding fully probabilistic, uncertainty-quantified corrections. Our workflow produces calibrated predictions for bandgaps, including credible intervals not only within the domain of existing data but also quantifies uncertainty for extrapolated predictions far from the training range. This approach delivers physically meaningful, interpretable results and provides a rigorous path to improve confidence in computational material screening and discovery. The methodology is directly extensible to a wide range of observables and DFT flavors, with future work set to further expand its scope and data-driven power.

**f0044**

**First–Principle Investigation of the Dynamical Stability, Electronic Structure, Mechanical, and Thermo-Physical Properties of the Ni3V Intermetallic Compound**

Dhvani Patel[1, *] Sujoy K. Choudhury[2] and K. Santhy[1]
[1]*Department of Materials and Metallurgical Engineering, IITE, Indus University, Ahmedabad, India 382115,*
[2]*Independent researcher, Paka Rasta More, Kalyan Nagar, Kolkata, 700112, India.*
**Correspondence author: dhwanipatel.jrf@indusuni.ac.in*

First principle calculation was performed to study the structural, mechanical, thermo-physical, electronic and dynamical properties of $Ni_3V$ intermetallic compound. The R phase and five possible geometrically closed pack structures-$D0_{19}$, $D0_{22}$, $D0_{24}$, $D0_a$ and $L1_2$ were considered to determine the most stable structure of compound. Based on the energy of formation and cohesive energy, $D0_a$ and $D0_{22}$ structure were found to exhibits nearly same stability. Among them, $D0_a$ is most stable, in this present study. The stable structure electronic, mechanic and thermo-physical were determined. The dynamic lattice stability of predicted structure was confirmed with phonon dispersion curve.

**f0045**

**First-principles calculations on Energetics of Rare-Earth Incorporation in Zircon ($ZrSiO_4$)**

Subhamoy Char[1, a)], K. Ali[1], and P. S. Ghosh[1,2]
[1]*Glass & Advanced Materials Division, Bhabha Atomic Research Centre, Mumbai 400 085, India*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai 400 094, India*
[a)] *Corresponding author: subhamoy.char2010@gmail.com*

The energetics of rare-earth element (REE) substituted zircon ($ZrSiO_4$) is investigated by combining classical molecular static and density functional theory (DFT) based calculations. The formation enthalpy ($\Delta H_f$) of $REE_xZr_{1-x}SiO_{4-x/2}$ solid-solutions (mechanism (1)) suggests their lack of stability at higher concentrations (x > 1/16). $REEPO_4$ exhibits a nearly linear trend in $\Delta H_f$ as a function of zircon concentration in $ZrSiO_4$-$REEPO_4$ solid solution (mechanism (2)) due the significantly higher energetic stability of $REEPO_4$ than $ZrSiO_4$. The $\Delta H_f$ for mechanism (2) is almost one order of magnitude higher than that of mechanism (1). The $REE^{3+}$-$V_O^{2+}$/$V_O^{2+}$-$V_O^{2+}$ clustering leading to the corner-shared $SiO_4$ tetrahedral chain formation and $REE^{3+}$-$PO_4^{3-}$ clustering is identified

as the REE solubility process in mechanism (1) and (2), respectively. Furthermore, chemical stability regime of $ZrSiO_4$ and $Zr_{(1-x)}Gd_xSi_{(1-x)}P_xO_4$ with x=0.25 is identified with respect to several possible competing phases.

**f0046**

**Formation Energy Prediction of 2D Materials Using Machine learning**

Fathimathul Afra K K[1,2], G. Tejaswini[2], Anjana E Sudheer[2], Amrendra Kumar[3,4], M. Vallinayagam[5,6], C. Kamal[3,4], M. posselt[7], M. Zschornak[5,6], D. Murali[2, a)]

[1]*Jamia Millia Islamia, Jamia Nagar, New Delhi-110025, India*

[2] *Indian Institute of Information Technology Design and Manufacturing Kurnool, Andhra Pradesh, India*

[3]*Theory and Simulations Laboratory, Theoretical and Computational Physics Section, Raja Ramanna Centre for Advanced Technology, Indore 452013, India*

[4]*Homi Bhabha National Institute, Training School Complex, Mumbai 400094, India*

[5]*IEP, TU Bergakademie Freiberg, 09599 Freiberg, Germany*

[6]*Fakultät Maschinenbau/Energietechnik/Physik, Hochschule für Technik und Wirtschaft 01069 Dresden, Germany*

[7]*Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research,01328 Dresden, Germany*

[a)]*Corresponding author: dmurali@iiitk.ac.in*

The rapid development of two-dimensional (2D) materials has spurred the need for efficient screening of new stable compounds. In this study, we employ machine learning (ML) techniques to predict the formation energy of 2D dichalcogen ($MXY$), dihalide ($MX'Y'$) and chalcohalide $MXX'$ (M = Sn, Pb, Sb, Bi; X/Y = O, S, Se, Te; X'/Y' = F, Cl, Br, I) single layers (SLs) using machine learning (ML). The geometry optimization of all the structures has been done by performing density functional theory (DFT) based calculations. The dataset contains a total of 144 SLs. We have analyzed the calculated formation energies and found that all the designed SLs are energetically favorable. We use the chemical properties of the elements as descriptors for the prediction. The simplest statistical learning method, linear regression is implemented on 80% of the data and the prediction has been made on the 20% testing data. The model is good in predicting the formation energy which is confirmed from the coefficient of performance $R^2$ being 0.75.

**f0047**

**Structural and vibrational insights into scheelite-type alkali metals of perrhenates (A= Na, K, Rb, Cs)**

Sathani Maddileti[1], Supratik Mukherjee[2], Alfonso Muñoz[3], Daniel Errandonea[4], Brendan J Kennedy[5], G Vaitheeswaran[1, a)]

[1] *School of Physics, University of Hyderabad, Prof. C. R. Rao Road, Gachibowli, Hyderabad-500046, Telangana, India*

[2] *Advanced Center of Research in High Energy Materials (ACRHEM), University of Hyderabad, Prof. C. R. Rao Road, Gachibowli, Hyderabad-500046, Telangana, India*

[3] *Departamento de Física, MALTA Consolider Team, Universidad de La Laguna, San Cristóbal de La Laguna, Tenerife E-38200, Spain*

[4] *Departamento de Física Aplicada ICMUV, MALTA-Consolider Team, Universidad de Valencia, Burjassot, Valencia 46100, Spain*

[5] *School of Chemistry, The University of Sydney, Sydney, New South Wales 2006, Australia*

[a)] *Corresponding author: vaithee@uohyd.ac.in*

This study investigates the structural, vibrational, and elastic properties of scheelite-type alkali-metal perrhenates, $AReO_4$ (A = Na, K, Rb, Cs), using first-principles calculations. The Na, K, and Rb compounds crystallize in a tetragonal structure, while $CsReO_4$ adopts an orthorhombic phase. Phonon and elastic analyses confirm both dynamic and mechanical stability, with phonon frequencies red shifting from Na to Cs. The low bulk and shear moduli indicate high deformability, which decreases with increasing ionic radius. High-frequency phonon modes are dominated by O and Re atoms, whereas low-frequency vibrations involve contributions from all atoms. The compounds also exhibit anisotropic pressure responses and ductile behavior.

**f0049**

**First-Principles Investigation of Ti-Doped 2D $MgH_2$: Electronic Structure, Phonon Stability, and Thermodynamic Properties.**

Jasveer Singh[1,a)] and Amarjeet Singh[b)]

[1)]*Department of Physics, Himachal Pradesh University, Summer Hill, 171005, Shimla*

[a)] *jasveerblp@gmail.com,* [b)] *amarjeet.sirohi@gmail.com*

We present a DFT-based study on the structural, electronic, and thermodynamic properties of 2D $MgH_2$ and its Ti-doped variant. The pristine 2D $MgH_2$ shows dynamic stability, as confirmed by positive phonon dispersion, and exhibits a wide band gap of 3.09 eV. Its formation enthalpy is calculated to be –54.36 kJ/mol, indicating strong thermodynamic stability. Upon substituting one Mg atom with Ti in a 3×3 supercell, the band gap reduces significantly to 0.42 eV, suggesting enhanced electronic conductivity. The partial density of states reveals dominant Ti 3d orbital contribution near the Fermi level. The doped system also shows a slightly reduced formation enthalpy of –48.78 kJ/mol, which may facilitate hydrogen desorption. These results demonstrate that Ti doping effectively tunes the electronic structure and thermodynamics of 2D $MgH_2$, making it a promising material for hydrogen storage applications.

**f0051**

**First-Principles Investigation of Pressure-Induced Half-Metallic Properties in RuMnIrZ (Z = Si, Ge, Sn) Quaternary Heusler Alloys**

Narayanan Namboodiri Puthusseri[1]and Baskaran Natesan[2]*
[1]*Department of Sciences and Humanities, J B Institute of Engineering and Technology, Hyderabad, India - 500075*
[2]*Condensed Matter Theory Laboratory, Department of Physics, National Institute of Technology, Tiruchirappalli-620015, India*
**Email: nbaski@nitt.edu.*

In the present work, we investigate the half-metallicity in RuMnIrZ (Z = Si, Ge, and Sn) quaternary Heusler alloys using density functional theory. Our results show that all alloys crystallize in the $F\bar{4}3m$ structure with a ferromagnetic ground state and negative formation energies, indicating experimental feasibility. The magnetic moments for RuMnIrSi, RuMnIrGe, and RuMnIrSn are 4, 4.004, and 4.033 μB, respectively, with the Mn atom contributing most to the total moment. While RuMnIrSi exhibits no half-metallicity despite a net integer magnetic moment, compressive pressure above 10 GPa induces half-metallicity in RuMnIrSi, which persists up to 25 GPa, after which it diminishes. RuMnIrGe and RuMnIrSn show no half-metallicity even under applied pressure. Elastic property calculations confirm the mechanical stability of the alloys, with RuMnIrSi and RuMnIrSn being ductile, and RuMnIrGe being brittle. RuMnIrSi, under appropriate pressure, emerges as a promising candidate for spintronics applications.

**f0052**

**Multi-Paradigm Comparative Study of H2 Ground and Excited State Potential Energy Curves Across Classical and Quantum Approaches**

Venkata Ramana Tadepalli, Golla Tejaswini and D Murali*
*Department of Sciences, Indian Institute of Information Technology Design and Manufacturing Kurnool Andhra Pradesh, 518007 India*
** dmurali@iiitk.ac.in*

The ground state potential energy curve (PEC) and the first three excited states of the hydrogen (H2) molecule are fundamental benchmarks in quantum chemistry, crucial for validating diverse computational methods. This study systematically investigates the H2 PEC across varying bond lengths using two distinct computational paradigms: classical ab initio quantum chemistry (Restricted Hartree-Fock (RHF), Unrestricted Hartree-Fock (UHF), and Full Configuration Interaction (FCI) via PySCF) and quantum simulations using the Variational Quantum Eigensolver (VQE) for ground states and Variational Quantum Deflation (VQD) for excited states, simulated with Qiskit. Classical methods demonstrate characteristic behaviors: RHF exhibits an unphysical dissociation limit, UHF provides a qualitatively better description at stretched bond lengths, and FCI serves as the exact reference for both ground and excited states within the chosen basis set. VQE and VQD simulations yield ground and excited state energies in close agreement with exact diagonalization, particularly near the equilibrium bond length, highlighting the promising potential of hybrid quantum algorithms for molecular energy calculations.

**f0053**

**Vertical heterostructures of ferroelectric BaTiO3 and topological insulator square tellurene**

G. Tejaswini[1], Anjana E Sudheer[1], Arwa Albar[2], S Assa Aravindh[3], M. Vallinayagam[4,5], M. Posselt[6], M. Zschornak[4,5], D. Murali[1, a)]
[1] *Indian Institute of Information Technology Design and Manufacturing Kurnool, Andhra Pradesh, India*
[2]*Department of Physical Sciences, Faculty of Science, University of Jeddah, PO Box 80327, Jeddah 21589, Saudi Arabia*
[3]*Nano and molecular systems research unit, University of Oulu, Pentti Kaiteran katu 1, Oulu 90570, Finland*
[4]*IEP, TU Bergakademie Freiberg, 09599 Freiberg, Germany*
[5]*Fakultät Maschinenbau/Energietechnik/Physik, Hochschule für Technik und Wirtschaft 01069 Dresden, Germany*
[6]*Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research,01328 Dresden, Germany*
*Email: *dmurali@iiitk.ac.in*

Herin, we design the BaTiO3-square tellurene (BTO-Te) van der Waals heterostructure (vdWH) and discuss its structural and electronic properties. BTO is the most studied oxide perovskite material which is explored for catalytic, piezoelectric, optoelectronic devices and multi-layer ceramic capacitors. On the other hand, square Te acts as a topological insulator which found applications in spintronics. The ultralow lattice mismatch between these layers will be promising for the design of the vdWH. We considered the two surface terminations for the BTO, the Ti- and Ba-termination. The binding energy of the designed vdWH has resulted in negative which indicates that the designed vdWH is energetically feasible. To date, the square Te monolayers have not been realized experimentally. The observed negative binding energy indicates that the BTO 001 surface can act as a good substrate for the growth of square Te. We have performed the electronic structure calculations including the spin-orbit coupling and observed metallic nature for the two surface terminations which will be promising for electronic device applications.

**f0054**

**Electrical Resistivity of Compound Forming Na-Pb Liquid Alloy**

S G Khambholja[1*], B Y Thakore[2] and A. Agraj[3]
[1]*Department of Science & Humanities, B & B Institute of Technology, Vallabh Vidyanagar, 388120, Gujarat, India*
[2]*Department of Physics, Sardar Patel University, Vallabh Vidyanagar, 388120, Gujarat, India*
[3]*Institute of Plasma Research, Gandhinagar, 382428, Gujarat, India*
**Email: physik.shyam@gmail.com (Email of corresponding author)*

The liquid alloys of alkali metals with lead are of great interest due to compound forming tendency. Sodium-Lead (Na-Pb) system is one of them. One of the features of compound formation is exhibited by a high value of electrical resistivity (~464 μΩ.cm in the case of Na-Pb); hence, a capable theoretical model should be able to reproduce results in its proximity. Well known theoretical model due to Faber and Ziman can not reproduce very high value of electrical resistivity and hence some modification is required to reproduce the correct resistivity isotherm. In the present work, we have coupled the model potential formalism with the t-matrix formulation. Finite phase shifts are calculated using a model potential instead of the Muffin-Tin (MT) potential. The effective valence is treated as a parameter to reproduce the experimental resistivity of pure Na and Pb. The results are in excellent agreement with the experimental results. Present results suggest that compared to the conventionally used approaches such as Faber-Ziman and 2kF scattering model, coupling model potential with t-matrix formalism can reproduce qualitative results of compound forming liquid alloys.

**f0057**

**High-Capacity Hydrogen Storage in Y-Decorated 2D Crystalline $C_2O$ Framework: Insights from DFT Simulations**

Muneeb Tariq[1,2,] Mala N Rao[1,2], B. Chakraborty[2, 3*]
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, INDIA*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai-400095, INDIA*
[3]*High Pressure & Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, INDIA.*
*a) Corresponding author: muneeb@barc.gov.in*

In our study, we investigated the practical hydrogen storage capabilities of a transition metal (Y) doped crystalline framework named $C_2O$. Density Functional Theory (DFT) calculations yielded an average $H_2$ adsorption energy of ≈ – 0.46 eV/$H_2$ and an average desorption temperature of 374.12K at 5 bar pressure. The $C_2O$ + Y system can adsorb up to five $H_2$ molecules per unit cell, achieving a gravimetric storage capacity of 10.28 wt%, which surpasses the US Department of Energy (DOE) target of 6.5%. Charge-transfer mechanism mediates the interaction between $H_2$ and the $C_2O$ + Y system wherein each Y atom loses a net charge of 0.94e to the $C_2O$ framework, computed by the aid of Bader analysis. The thermodynamic stability was confirmed by ab initio molecular dynamic simulation at 300 K and dynamic stability by computing phonon spectrum with positive phonon frequencies.

**f0058**

**The Impact of Dual-Fluid Saturation on the Dispersion of SH-Waves in Geological Porous Medium**

Rajbir Kaur[1, a)] and Ashish Arora[2]
[1]Applied Sciences Department, Guru Nanak Dev Engineering College, Ludhiana-141006, Punjab, India.
[2]*Department of Mathematical Sciences, IKG Punjab Technical University, Kapurthala-144 603, Punjab, India.*
[a)] *Corresponding author: rajbiramar@yahoo.com*

This paper investigates the SH-wave propagation in the porous layer saturated by two fluids and lying over an elastic half-space. The impacts of various fluid saturations in the porous layer are examined to understand how they collectively affect the dispersion characteristics of SH-waves. The dispersion relation of the SH-wave using suitable boundary conditions is derived. The numerical analysis shows that the different fluids in the porous layer significantly affect the phase speed of the SH-wave.

**f0060**

**Crystallinity and Structural Properties of Tussar and Bivoltine Silk Fibers through X-ray Diffraction [XRD]: A Comparative Study**

Ranjitha. K[1]. V. Annadurai[2], Ritu Tomar[3]
[1]*Nitte Meenakshi Institute of Technology, Nitte (Deemed to University), Bangalore, India.*
[2]*NIE First Grade College, Mysore, India*
[2,3]*Department of Physics, Sambhram Institute of Technology, Bangalore, India*
*k.ranjitha@nmit.ac.in*

This study investigates the effect of irradiation on the crystalline and structural properties of Tussar and Bivoltine silk fibers using X-ray diffraction (XRD) analysis. Descriptive statistics (Tables 1 and 2) revealed that while the primary diffraction peak (2θ ≈ 20–21°) remained unchanged, significant differences in diffraction intensity were observed between the control and irradiated samples. Tussar silk displayed a marked reduction in crystallinity and crystallite size after 5 min irradiation, with only partial recovery at 10 min. In contrast, Bivoltine silk maintained a stable crystallite size and exhibited enhanced diffraction intensity and reduced lattice defects at higher exposure, indicating irradiation-induced molecular reorganization. The crystallographic parameters (Table 3), including crystallite size, d-spacing, microstrain, and dislocation density, confirmed these observations, with Bivoltine silk showing greater structural resilience compared to Tussar silk. Williamson–Hall plots (Figure 2) further demonstrated that Bivoltine silk accommodated irradiation effects through reduced lattice strain and improved lattice perfection at 10 min exposure.

**f0061**

**Pressure And Strain Induced Modification In Thermoelectric Behavior of Half Heusler Alloy, HfNiSn**

Komal Verma[1], Pawan Kumar singh[2,3], Rishi Pal Singh[2,3] and Arvind Kumar[1,*]
[1]*School of Physical Science, Jawaharlal Nehru University, New Delhi-110067 (India)*
[2]*Department of Physics, S.S.V. College, Hapur, Uttar Pradesh- 245101 (India)*
[3]*Deaprtment of Physics, CCS University, Meerut, Uttar Pradesh-250001 (India)*

**Email:avind@jnu.ac.in*
Effect of pressure and strain has been studied on half Heusler (HH), HfNiSn for its thermoelectric behaviour using first principles calculations. Density of state and band structure profile shows the narrow indirect bandgap of $\sim 0.36\ eV$. zT parameter is calculated to be ~ 0.74 at room temperature. zT parameter is found to be ~ $0.82$ and $0.81$ at ~ $300K$ for $-10GPa$ and $10GPa$, respectively and zT value is approaching $1$ in case of $-4\%$ strain at lower temperature (below 300K). Overall, study reveal that HfNiSn proves to be a good thermoelectric material at lower temperature with application of applied pressure and strain.

**f0063**

**Multiply-charged Weyl and Triple Point Phonons in $Pd_3(PbS)_2$ Compound: A First-principles Calculations**

Jay Panchal, Saurav Patel and Prafulla K. Jha

*Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, India-390002*

**Email: jaypanchal831@gmail.com*

Topological phonons with nonzero invariants have attracted interest for hosting unconventional phenomena. However, materials exhibiting multiple phonon types with distinct topological charges remain rare. In this work, using first-principles calculations we identify the chiral cubic compound $Pd_3(PbS)_2$ as a realistic material platform in which two distinct types of topological phonons coexist: charge-1 Weyl points (WPs) and charge-2 triple points (TPs). We computed Chern numbers via the Wilson loop method and analyzed the associated surface states. Our results reveal that these topological band-crossing points occur at high-symmetry locations within the frequency range of 53–61 THz, where the phonon spectrum exclusively consists of the bands responsible for these crossings. The surface phonon arcs form extended paths in momentum space, connecting WPs and TPs across the Brillouin zone. This unique connectivity enhances the prospects for experimental detection through techniques such as inelastic neutron scattering or high-resolution electron energy loss spectroscopy. Our findings establish $Pd_3(PbS)_2$ as a promising platform for the study of multiple topological phonon excitations within a single material system.

# g) Dielectric, ferroelectric and piezoelectric materials

**g0002**

**Study of Hysteresis Scaling Exponent Behavior in Fe Modified $BaTiO_3$**

Shivani Kulasari [1*], Ayush Rana[1], Meenal Dhanetwal[2], Sapan Kumar[1], V.R. Reddy[2], Sanjay Kumar Upadhyay[1]
[1]*HNB Garhwal University Srinagar-Garhwal-246174, Uttarakhand, INDIA*
[2]*UGC-DAE Consortium for Scientific Research, Khandwa Road, University Campus, Indore-452 001, INDIA*
**Email: kulasaris@gmail.com*

In the present work, ferroelectric hysteresis dynamics have been studied for Fe-modified Barium titanate (BaTi0.98Fe0.02O3). A comparative study has been carried out with respect to the behavior of the internal bias field present in the sample. The cause of ageing in the present sample is due to the charge imbalance between Fe3+ and Ti4+. We have studied the hysteresis scaling exponent behavior by considering $< A > \propto E^n$ and $< A > \propto (E + Ei)^n$, respectively, where A is the area of the hysteresis curve, E is the applied field, and Ei is the internal bias field. It has been found that the relation $< A > \propto (E + Ei)^n$ holds for aged samples.

**g0004**

**Role of $V_2O_5$ in Modifying the Sintering Kinetics and Electrical Characteristics of Lead-Free BNT-BT-KNN Ceramics**

Kiran Kumar Padhi and Swarup Kundu
*Sri Sathya Sai Institute of Higher Learning, Prashanti Nilayam Campus, Andhra Pradesh-515134*
**Email: swarupkundu@sssihl.edu.in*

In pursuit of sustainable alternatives to lead-based piezoelectrics, this study investigates the effect of vanadium pentoxide ($V_2O_5$) as a sintering aid on the structural, microstructural, and electrical properties of lead-free $Bi_{0.5}Na_{0.5}TiO_3$–$BaTiO_3$–$K_{0.5}Na_{0.5}NbO_3$ (BNT-BT-KNN) ceramics. Samples were synthesized via the conventional solid-state route with varying $V_2O_5$ concentrations (0–1.0 wt%) and sintered at optimized temperatures. X-ray diffraction (XRD) confirmed a stable perovskite structure within the morphotropic phase boundary (MPB), while scanning electron microscopy (SEM) revealed enhanced densification and refined grain morphology at low $V_2O_5$ content. Dielectric analysis indicated a maximum dielectric constant near 400 °C, with frequency-dependent behavior. The 0.1 wt% $V_2O_5$-doped sample exhibited the highest density (5.15 g/cm³) and optimal dielectric performance with low loss (tan δ < 1). P–E hysteresis loops confirmed the ferroelectric nature of all compositions, with the 1.0 wt% $V_2O_5$ sample showing the highest polarization ($P_{max}$ = 9.34 μC/cm²). These findings demonstrate that controlled $V_2O_5$ addition significantly tailors the sintering behavior and enhances the piezoelectric potential of BNT-BT-KNN ceramics for lead-free energy and sensor applications.

**g0005**

**Probing the multiferroic Response of Brownmillerite-Based Composite Through Thermal and Magnetic Field Perturbation**

D.P. Sahu[1]. A. Mohanty[1], G. Palai[1], C. Mahapatra[1], A. K. Singh[1, *]
*Department of Physics and Astronomy, National Institute of Technology Rourkela, Odisha 769008, INDIA*
**Email: singhanil@nitrkl.ac.in*

This study investigated the magnetic, dielectric and magnetodielectric (MD) properties of a 0.9KBFO-0.1NFO composite synthesized using the sol-gel method. The dielectric constant and storage properties were characterized across a broad temperature range of 30 to 580 °C, revealing a maximum dielectric constant of $15.13\times10^3$. Temperature- and field-dependent magnetic measurements were conducted to ascertain the magnetic properties, confirming the presence of finite magnetic parameters. The magnetodielectric coupling and loss characteristics were thoroughly examined using three different analytical techniques at different frequencies.

**g0007**

**A Comprehensive study on the structural, magnetic, and Dielectric Characteristics of $Bi_2Fe_4O_9$/$NiFe_2O_4$ Composite**

A. Mohanty[1], D.P. Sahu[1], G. Palai[1], C. Mahapatra[1], A. K. Singh[1, *]
*Department of Physics and Astronomy, National Institute of Technology Rourkela, Odisha 769008, INDIA*
**Email: singhanil@nitrkl.ac.in*

The composite $0.9Bi_2Fe_4O_9/0.1NiFe_2O_4$ was synthesized via the sol–gel auto-combustion method, and its structural, magnetic, and dielectric properties were systematically investigated in the present work. Rietveld refinement of room-temperature (RT) X-ray diffraction (XRD) patterns confirmed the coexistence of dual-phase formation. The microstructural analysis indicated non-uniform grain dispersion, with the average grain size estimated to be around ~ 0.5μm. The RT M–H curve of the composite exhibited low saturation magnetization of ~5 emu/g under an applied field of ±15 kOe. Temperature-dependent magnetization shows the Curie transition of the composite around ~ 830 K. Dielectric measurements as a function of temperature at constant frequencies showed an anomaly near 300 K, indicating magnetodielectric (MD) coupling. The presence of MD coupling enhances the potential of the composite for multifunctional applications such as memory devices, sensors, and actuators.

**g0008**

**Signatures Of Atomic Displacement Leading to Ferroelectricity In Multiferroic $TbMnO_3$: A Polarized Raman Study**

Pragati Sharma[1], Divya Jangra[1], Binoy K. De[1,2], Ajay Rathore[1] and Vasant G. Sathe[1, a)]
[1]*UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, India*
[2]*Centre for Nano Science and Engineering, Indian Institute of Science, Bangalore-560012, India*
[a)] *Corresponding author: vasant@csr.res.in*

$TbMnO_3$ is a prototypical material with type-II multiferroic behavior presenting huge magneto-electric coupling where ferroelectricity can be manipulated by applying magnetic field. The ferroelectricity shown by this compound under zero field is reflected in the form of a transition below 28 K which is attributed to femtometer scale ionic displacement from the centro-symmetric position. Here, we present our detailed polarized Raman spectroscopy study and provided direct evidence of ionic displacement along c-axis by employing a unique protocol invented in our laboratory. Under this protocol vibrational properties and symmetry of the crystal lattice with respect to polarization of the incident light is used to analyze changes in the Raman tensor elements. In the present study, these variations manifest as distinct variation in intensity of specific Raman-active modes across ferroelectric transition providing direct evidence of femtometer scale atomic displacement as the root cause for the ferroelectric transition shown by this system.

**g0009**

**Energy Tunable Anisotropic Light Matter Interaction in Ferroelectric In2Se3**

Divya Jangra[1,] Pragati Sharma[1,] Binoy Krishna De[1,2,] Praveen Kumar Velpula[1] and Vasant G. Sathe[1, a)]
[1]*UGC-DAE Consortium for Scientific Research. University Campus, Khandwa Road, Indore-452001, India*
[2]*Cente for Nano Science and Engineering, Indian Institute of Science, Bangalore-560012, India*
[a)] *Corresponding author: vasant@csr.res.in*

The study of anisotropic light-matter interaction in 2D materials is gaining attention due to its potential for futuristic light polarization-based optoelectronic applications. The anisotropic structure of these 2D materials is responsible for their anisotropic light-matter interaction. In this work, we have studied the light polarization-dependent light-matter interaction in ferroelectric 3R α-$In_2Se_3$ using Angle-Resolved Polarized Raman Spectroscopy (ARPRS) with different excitation lasers. The study showed that the anisotropy in optical properties is not only depends on the structural anisotropy but it depends on the wavelength of the incident light. The anisotropic response in the Raman study can be fitted only when complex Raman tensor elements are considered which have different values for different wavelengths. The results are explained by invoking the complex interplay of electron-photon and electron-phonon interactions.

**g0011**

**Spin, Lattice, and Pressure Effects in $LuFeO_3$: Experimental and Theoretical Approach**

Sourav Bag[1], Samiran Malgope[1,2,] Mayanak K Gupta[1,2], Ranjan Mittal[1,2], Sanjay K Mishra[1,2], Stephane Rols[3], and Samrath L Chaplot[1,2]
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400085, India*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*
[3]*Institut Laue-Langevin, BP 156, 38042 Grenoble Cedex 9, France*
*Email: bsourav@barc.gov.in*

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.

**g0012**

**Signature of Stacking Faults and Dislocations in Single Crystal Neutron Diffraction data of Tris-Sarcosine Calcium Bromide**

Rajul Ranjan Choudhury[1,2], R. Chitra[1]
[1] *Solid State Physics Division, Bhabha Atomic Research Center, Trombay Mumbai, India 400085*
[2] *Homi Bhabha National Institute, Mumbai, India 400085*
**rajul@barc.gov.in*

Tris-sarcosine Calcium chloride (TSCC) is a very well-studied hydrogen bonded ferroelectric crystal, Tris-sarcosine Calcium bromide (TSCB) is isostructural to TSCC. These crystals exhibit ferroelastic behaviour at room temperature. These crystals are almost aways twinned with (0 1 1) and (0 3 1) planes acting as twin planes. We have performed single crystal neutron diffraction investigations on TSCB, we report here the effects of twinning on the peak shapes of Bragg reflections recorded from a TSCB crystals.

**g0014**

**A-site Disordered High-Entropy Perovskite Ceramics for Energy Storage Applications**

Kishor Kalita[1], Shashi Priya Balmuchu[2], Pamu Dobbidi[2] and Mahesh Peddigari[1, a)]
[1]*Indian Institute of Technology Hyderabad (Department of Physics, IIT Hyderabad, Hyderabad, India)*
[2]*Indian Institute of Technology Guwahati (Department of Physics, IIT Guwahati, Guwahati, India)*
**Email: mahesh.p@phy.iith.ac.in*

Dielectric capacitors have received significant interest for advanced pulsed power applications due to their capability to deliver high power densities and rapid charge-discharge cycles. Unlike batteries, which offer high energy densities but lower power output, dielectric capacitors are limited by their relatively low energy storage capacities, restricting their broader application in modern electronic devices. This study presents a single-phase $BaTiO_3$-based high-entropy (BNBSCT) ceramic, which is synthesized using

a conventional solid-state reaction method. The BNBSCT ceramic exhibits a remarkable energy storage performance, with a $W_{rec}$ of 188 mJ/cm$^3$ and an efficiency of 70% at 45 kV/cm electric field. The study reveals that the introduction of high entropy concept enhances the lattice distortion and sluggish diffusion effect in the high entropy ceramics, which in turn enhances the breakdown strength and energy storage density of the capacitors.

**g0015**

**Dielectric, Impedance, and Electrical Conductivity Analysis of $BaZr_{0.1}Ti_{0.9}O_3$ Electroceramics**

Saurabh Kumar Mishra, Subhasis Sarangi, and P. M. Sarun*
*Functional Ceramics Laboratory, Department of Physics, Indian Institute of Technology (Indian School of Mines), Dhanbad 826004, India.*
**Corresponding author: sarun@iitism.ac.in*

In the present study, a solid-state reaction approach was used to synthesize $BaZr_{0.1}Ti_{0.9}O_3$ (BZT). XRD analysis showed the presence of a single-phase tetragonal structure with *P4mm* symmetry. FE-SEM investigation showed a homogeneous microstructure with an average grain size of almost 1.86 µm. Dielectric study revealed significant temperature and frequency dependency, mainly due to space charge polarization effects. Extremely low tangent loss and electrical conductivity indicate excellent charge storage with minimal energy dissipation. The high impedance value indicates that it is suitable for memory devices and high-performance capacitors.

**g0016**

**Study of Dielectric & Ferroelectric Behavior in Mn Modified $BaTiO_3$**

Ayush Rana1, a), Shivani Kulasari, Rony Kohli, Piyush Singh, Om Prakash, and Sanjay Kumar Upadhyay
*HNB Garhwal University Srinagar-Garhwal-246174, Uttarakhand, INDIA*
**Email: ayushrana161002@gmail.com*

In the present work, Mn-doped barium titanate, $BaTi_{1-x}Mn_xO_3$ (x=0.02, 0.05), was studied by means of x-ray diffraction, ferroelectric, and dielectric measurements. Phase-coexistence (tetragonal and hexagonal) has been observed for both compositions. For x= 0.02, a pinched type of ferroelectric hysteresis loop has been observed due to the presence of defect dipole. The origin of the defect dipole can be understood in terms of the generation of oxygen vacancies, created by the charge imbalance of $Ti^{4+}$ and $Mn^{3+}$. The transition temperature for x= 0.02 sample comes out to be 395 K. For x= 0.05 sample, typical paraelectric behavior has been observed in PE loop at room temperature. However, the transition temperature comes out to be 391 K in temperature-dependent dielectric data, essentially associated with a small fraction of tetragonal phase.

**g0018**

**Flexible High-Performance Nanogenerator for Self-Powered Pressure Sensors Using $BaTiO_3$/PVDF**

Chetna[1], Mukul Kumar[1], Jaspal Singh[2], Deepak Kumar Sharma[3], Sanjeev Kumar[1, a)]
*[1]Physics Department, Punjab Engineering College (Deemed to be University), Chandigarh -160012, India*
*[2]Department of Physics, Punjabi University, Patiala, 147002, India*
*[3]Electronics and Communication Engineering Department, Punjab Engineering College (Deemed to be University), Chandigarh - 160012, India*
**Email: sanjeev@pec.edu.in*

Flexible piezoelectric nanogenerators (PENGs) have become promising sustainable power sources for self-powered wearable electronics by converting ambient mechanical energy into electricity. In this work, we present a lead-free PENG device based on a $BaTiO_3$ (BTO) nanoparticle-embedded polyvinylidene fluoride (PVDF) nanocomposite film. Dielectric measurements revealed a significant increase in dielectric constant from 8.1 to 15.6 with BTO addition. Polarization-electric field (P–E) measurements confirmed enhanced ferroelectric behavior, with the PVDF/3 wt% BTO composite exhibiting a spontaneous polarization ($P_s$) of ~ 0.76 µC/cm² and enhanced efficiency of 67.6% at 300 kV/cm. The potential of fabricated PENG being used for energy harvesting applications was demonstrated by the fact that it provided an output voltage of ~15 V when it was tapped with the finger.

**g0020**

**Magneto-electric Coupling In CZFMO-Embedded P(VDF-TrFE) Composites For Self-powered Electronics and Magnetic Energy Scavenging**

Jasveer Singh[1], Kirti Dutta[1], Jaspal Singh[1,a]
*[1]Department of Physics, Punjabi University, Patiala-14002, Punjab, India*
*[a] Corresponding Author: jaspal_phy@pbi.ac.in*

The present research focuses on the development and characterization of $Co_{0.6}Zn_{0.4}Fe_{1.7}Mn_{0.3}O_4$ (CZFMO)-embedded poly(vinylidene fluoride-trifluoroethylene) [P(VDF-TrFE)] composites for magnetic energy harvesting applications. Initially, the structural and vibrational properties of the composites were analyzed using X-ray diffraction (XRD) and Fourier-transform infrared (FTIR) spectroscopy, respectively. Subsequently, dielectric measurements were performed to evaluate the dielectric constant and loss behavior of the composites. Among the samples, the composite containing 0.5 wt.% CZFMO exhibited an appreciable magnetoelectric (ME) voltage coefficient of 52.31 mV/(cm·Oe). Finally, the energy harvesting capability of the optimized composite was investigated. The output voltage demonstrated a proportional response to increasing magnetic field strength, rising

from 0.3 V to 0.9 V as the applied magnetic field increased from 0.9 mT to 2.7 mT. These results highlight the potential of CZFMO/P(VDF-TrFE) composites in low-field magnetic energy harvesting applications.

**g0021**

**Microstructure–Property Correlation in Microwave-Sintered NBSTS-BT Ceramics for Enhanced Dielectric Energy Storage**

*Varun Kamboj[1], Shubham Modgil[1], Mukul Kumar[1], Arun Kumar Singh[2], Sanjeev Kumar[1*]*
*[1]Physics Department, Punjab Engineering College (Deemed to be University), Chandigarh 160012, India*
*[2]Electronics and Communication Engineering Department, Punjab Engineering College (Deemed to be University) Chandigarh 160012, India*
*[*]Email: sanjeev@pec.edu.in; sanjeev04101977@gmail.com*

The pursuit of sustainable and efficient dielectric materials has steered attention toward lead-free ferroelectric ceramics. Developing high-performance lead-free dielectrics remains a central challenge due to the difficulty of achieving multifunctional performance metrics in a single material system. In this study, innovative processing of $0.94(Na_{0.5}Bi_{0.5})_{0.75}Sm_{0.25}Ti_{0.95}Sc_{0.05}O_3$–$0.06BaTiO_3$ ceramics through microwave sintering significantly enhances energy storage behavior. Under a high field of 221.5 kV/cm, the microwave-sintered ceramics achieve high recoverable energy density ~0.93 J/cm³ and high η ~80.86%, outperforming conventionally sintered counterparts. FESEM micrographs indicate dense and uniform microstructure of MS ceramics. A high dielectric constant ~1600 and ~ 1100 is observed for CS and MS ceramics, respectively. These findings suggest microwave sintering as a rapid and efficient route to enhance energy storage performance.

**g0022**

**Microwave-Assisted Sintering of KNN-Based Relaxors: Local Structure Homogeneity and Nanodomain Engineering for High Energy Storage Efficiency**

Twinkle[1], Mukul Kumar[1], Shubham Modgil[1], Arun Kumar Singh[2], Sanjeev Kumar[1 a)]
*[1]Physics Department, Punjab Engineering College (Deemed to be University), Chandigarh -160012, India*
*[2]Department of Electronics and Communication Engineering, Punjab Engineering College (Deemed to be University), Chandigarh -160012, India*
*[a)]Email: sanjeev@pec.edu.in*

Microwave sintering represents an advanced technological innovation that significantly accelerates the synthesis process in bulk ceramics, thereby enhancing time efficiency. In this paper, we have synthesized $0.875K_{0.5}Na_{0.5}NbO_3$-$0.125Bi(Zr_{0.98}Sr_{0.02})O_3$ via conventional as well as microwave sintering and analyzed both for the energy storage properties. XRD Refinement demonstrates the structure to be tetragonal with P4mm symmetry. Dielectric studies with temperature reveal the dielectric properties of the samples. $\varepsilon_{max} \sim 1481$ was observed in conventional sintered sample with $T_m$~ 405℃. FESEM studies implies that grain size of ceramics obtained via microwave sintering is finer as compared to that of conventional sintering. This, eventually, enhanced the breakdown strength of microwave sintered sample. Ferroelectric properties investigated via P-E loops signifies slim nature with high maximum polarization $P_{max} \sim 20\ \mu C/cm^2$,low remnant polarization, $P_r \sim 3\ \mu C/cm^2$ and hence high recoverable energy density $W_{rec}$~ 0.89 J/cm$^3$ with 70 % efficiency in microwave sintered sample. Hence, this study demonstrates the potential use of microwave in enhancing the energy storage capabilities of bulk ceramics.

**g0023**

**Structural and Frequency-Dependent Dielectric Properties of $HfO_2$ & Sr-doped $HfO_2$ Ceramics Synthesised Via Hydrothermal Method for Energy Applications**

Rajib Basumatary[1] and Rajeeb Brahma[1, a]
*[1]Department of Physics, Bodoland University, Kokrajhar, Assam-783370, India*
*[a)] Email: rajibhcu@gmail.com*

$HfO_2$ and Sr-doped $HfO_2$ nanoparticles were synthesized via the hydrothermal method and subsequently calcined at 500°C for 5 hours. X-ray diffraction analysis confirmed the formation of an orthorhombic phase with space group Pbcm. Photoluminescence spectra reveal the presence of defects and radical species. The dielectric measurement at room temperature revealed a high dielectric constant with low dielectric loss. Nyquist plot of ceramics shows the significant grain boundary contributions to the impedance behavior. The AC conductivity analysis ($\sigma_{ac}$) reveals that the dominant charge transport mechanism is governed by hoping mechanism.

**g0024**

**Structural, Dielectric, and Impedance Analysis of $BaTi_{0.95}Sn_{0.05}O_3$ Ceramics for MLCC Applications**

Subhasis Sarangi, Saurabh Kumar Mishra, and P. M. Sarun*
*Functional Ceramics Laboratory, Department of Physics, Indian Institute of Technology (Indian School of Mines), Dhanbad 826004, India*
**Email: sarun@iitism.ac.in*

In this study, $BaTi_{0.95}Sn_{0.05}O_3$ (BST) ceramic was synthesized via the solid-state reaction method. The Rietveld refinement pattern confirmed the presence of a single-phase tetragonal structure. FE-SEM image revealed an average grain size of nearly 0.522 µm with some porosity. Dielectric studies showed a strong frequency and temperature dependence, attributed to space charge

polarization effects. Impedance spectroscopy and Nyquist plots revealed distinct contributions from grain and grain boundaries, with the grain boundary resistance significantly higher. Electrical conductivity demonstrated a transition from dc to ac conductivity, indicating hopping conduction mechanisms that are thermally activated.

**g0025**

**Frequency dependent Dielectric and Impedance analysis of Bismuth Ferrite Ceramics at Room Temperature**

Sujeet Kumar, Saurabh Kumar Mishra, P M Sarun*
*Department of Physics, Indian Institute of Technology (ISM), Dhanbad– 826004, India.*
**Corresponding author: sarun@iitism.ac.in*

This study presents a comprehensive investigation of the structural, microstructural, dielectric, and impedance characteristics of pure-phase $BiFeO_3$ ceramics synthesized via conventional solid-state reaction. X-ray diffraction analysis confirms the formation of rhombohedral phase perovskite structure with space group *R3c*, while field emission scanning electron microscopy reveals densely packed, irregularly shaped grains with minor porosity. Frequency-dependent dielectric and impedance spectroscopy measurements exhibit dispersion behavior and non-Debye-type relaxation, indicative of heterogeneous electrical response. The conduction mechanism is predominantly governed by space charge polarization and interfacial effects at grain boundaries. These findings show the intrinsic correlation between the microstructural features and the electrical transport properties, reinforcing the potential of $BiFeO_3$ ceramics for multifunctional applications.

**g0026**

**Piezoelectric KNN-Nylon 11 Composites: A Step Towards Clean Energy and Green Electronics**

Vinatha Ashokan[1] and Nijesh K. James[1*]
[1]*Department of Physics, St. Joseph's College (Autonomous) Devagiri-673008, Affiliated to University of Calicut, Kerala, India.*
**Email: nijeshkjames@gmail.com*

The pursuit of sustainable, lead-free piezoelectric materials is critical for advancing flexible electronics and energy harvesting technologies in line with global sustainability targets. In this study, we present the fabrication and characterization of potassium sodium niobate (KNN)–Nylon 11 composites, engineered to combine mechanical flexibility with enhanced piezoelectric and dielectric functionality. Composites with varying KNN concentration (0-50%) was fabricated via melt bending and hot-pressing techniques. Structural integrity was confirmed via XRD and SEM analyses, revealing uniform filler dispersion and phase retention. Piezoelectric and dielectric studies revealed a notable enhancement in piezoelectric properties and permittivity with increasing ceramic content, attributed to interfacial polarization and micro capacitive effects. Ferroelectric hysteresis (P–E) loop measurements demonstrated a transition from non-switching dielectric behavior at lower filler content (10–20 vol%) to well-defined ferroelectric loops at 30–50 vol%, highlighting the active role of KNN in inducing polarization switching. The composite with 40 vol% KNN exhibited optimal performance, with enhanced remanent polarization and coercive field, suggesting potential for energy harvesting applications. The study presents a scalable route to developing flexible, lead-free piezoelectric materials, combining the mechanical flexibility of polymers with the functional properties of ceramics, making them suitable candidates for wearable and portable electronic devices.

**g0027**

**The Structural and Dielectric Properties of Gd Doped Double Perovskite $Y_{2-x}Gd_xCoMnO_6$**

Rosmy Jose[1] and Shinto P Mathew [2]
*Department of Physics, St. Joseph's College (Autonomous), Devagiri, Calicut 08, India*
**Email: rosmyjose11193@gmail.com*

In this contribution, the structural, dielectric, and microstructural properties of perovskite $Y_2CoMnO_6$ doped with gadolinium are presented. The gadolinium doped double perovskite $Y_{2-x}Gd_xCoMnO_6$ (x=0.00, 0.02, 0.04, 0.06, 0.08) were prepared by solid state reaction method intending to tune the dielectric properties of multiferroic $Y_2CoMnO_6$. The Rietveld refinement study exhibited the pure phase formation with orthorhombic pnma space group. A decrease in crystallite size and grain size is noted with doping of gadolinium to yttrium site. The induced strain arose with gadolinium doping, is employed with Williamson Hall Plot. A detailed temperature and frequency dependent dielectric spectroscopic studies revealed enhancement in dielectric constant and reduction in dielectric loss factor with gadolinium doping. Impedance spectroscopic studies are also carried out. Temperature variation of the frequency exponent shows the possible conduction mechanisms like small polaron tunneling, quantum mechanical tunneling and carrier barrier hopping existing in each sample. High dielectric permittivity with low loss factor makes $Y_{2-x}Gd_xCoMnO_6$ a promising candidate to develop high dielectric constant materials.

**g0029**

**Structural Phase Transition in $K_xNa_{1-x}NbO_3$**

Abhisikta Sahu,[1] Anupam Mishra,[2] Md. Mijanur Rahaman,[3] Dillip Kumar Pradhan[1, a)]
[1]*Department of Physics and Astronomy, National Institute of Technology, Rourkela, Odisha 769008, India.*
[2] *Department of Ceramic Engineering, National Institute of Technology, Rourkela, Odisha 769008, India.*
[3]*Department of Materials Science and Engineering, University of Rajshahi, Rajshahi 6205, Bangladesh*
*a) Corresponding author: dillip.pradhan79@gmail.com*

Lead-free ferroelectric ceramic oxides; $K_xNa_{1-x}NbO_3$ ($x$ = 0.45, 0.50 and 0.55) have been prepared using solid-state reaction technique by varying K/Na ratio. Their crystal structures have been investigated using XRD and Raman spectroscopic techniques at room temperature (RT). Rietveld refinement analysis on XRD data suggest the monoclinic crystal structure having P*m* space group for $K_{0.45}Na_{0.55}NbO_3$ and orthorhombic crystal structure with A*mm2* space group for both $K_{0.5}Na_{0.5}NbO_3$ and $K_{0.55}Na_{0.45}NbO_3$ respectively. The composition driven structural phase transition of the $K_xNa_{1-x}NbO_3$ is seen by the splitting of the mode near 191 $cm^{-1}$ as well. The presence of prominent central peak (CP) reveals the order-disorder nature of the ferroelectric phase transition of the $K_xNa_{1-x}NbO_3$.

**g0030**

**Structural, Mechanical and Dielectric Characteristics of $Li_2O$-$GeO_2$-$SiO_2$-$Al_2O_3$ Glass Ceramics Doped with $TiO_2$**

Suresh Suragani[1], M. V. Sambasiva Rao[2], Ch. Tirupataiah[3 a)], Bhavani Naga Prasanna. H[1], and M. Naga Lakshmi[2]
[1]*Department of Basic Sciences and Humanities, Vignan's Nirula Institute of Technology and Science for Women, Peda Palakalur, Guntur, Andhra Pradesh, 522009, India.*
[2]*Bapatla Engineering College, Bapatla -522101, A.P., India.*
[3]*Department of Physics, School of Applied Science and Humanities, Vignan Foundation for Science, Technology, and Research, Guntur, Andhra Pradesh 522213, India.*
[a)] *Email: chereddyt@gmail.com (Email of corresponding author)*

Glass ceramics with composition $25Li_2O$-(10-x) $GeO_2$-$60SiO_2$-$5Al_2O_3$-x$TiO_2$ (x=1–5 mol%) were synthesized by melt quenching. XRD revealed various crystalline phases, which were confirmed by SEM. EDS analysis confirmed the elemental composition. Vickers hardness increased from 8.80 GPa (T1) to 24.59 GPa (T5) due to $TiO_2$ nucleation, denser microstructure, and stronger Ti–O bonds. FT-IR spectra showed bands at 400–1600 $cm^{-1}$ for O-Si-O bending, $TiO_4$ vibrations, Ge-O-Ge stretching, and Si-O-Si modes. Dielectric studies indicated frequency-dependent decreases in real (ε') and imaginary (ε") permittivity. T5 displayed high ε' and low ε" suitable for capacitors, transducers, and microwaves, while T3's low ε' fits low-k applications; $TiO_2$ doping enhances mechanical and electrical performance amid $GeO_2$ reduction.

**g0031**

**Structural Characteristics and Dielectric Features of Lead-Free BKT-BST Submicrorods**

Shweta S. Watile[1], Ajay B. Lad[1,2a)], Anand S. Kakde[1], Shahin K. Sayyad[3], Vishwajit M. Gaikwad[1b)]
[1] *Department of Physics, Amolakchand Mahavidyalaya, Yavatmal 445001, Maharastra, India.*
[2]*Innovation, Incubation and Linkages (IIL) Centre, S. G. B. Amravati University, Amravati 444602, India*
[3]*Shri Shivaji Science College, Congress Nagar, Nagpur 440012*
Corresponding authors: [a)] drajay_lad@rediffmail.com, [b)]vish9823@gmail.com

In the present work, the synthesis protocol, structural and dielectric properties of lead-free submicrorods of $0.75Bi_{0.5}K_{0.5}TiO_3$-$0.25Ba_{0.5}Sr_{0.5}TiO_3$ (BKT-BST) are presented. Structural study confirms tetragonal structure with slight distortion in $TiO_6$ octahedra. Morphological analysis indicates the formation of highly dense submicrorods. Room temperature dielectric spectra show that the BKT-BST submicrorods exhibits significant dielectric constant with low dissipation, making them a potential candidate for microelectronics application.

**g0032**

**Influence of α-$Fe_2O_3$ Nanoparticles on the Structural, Physical and Optical Properties Doped Zinc Telluroborate Glasses**

Preethi H[1], Devaraja C[1, a)], Ambika M R[2], Utpal Deka[3]
[1]*Department of Physics, Manipal Institute of Technology Bengaluru, Manipal Academy of Higher Education, Manipal, India*
[2]*Department of Physics, M S Ramaiah Institute of Technology, MSR Nagar, Bengaluru 560054, India*
[3]*Department of Physics, Sikkim Manipal Institute of Technology, Sikkim Manipal University (SMU), Majitar, India*
[a)] *Corresponding author: devaraja.c@manipal.edu*

The influence of α-$Fe_2O_3$ nanoparticles on the physical, structural, optical characteristics of the produced glass with the formula (68-x)$B_2O_3$+$15TeO_2$+$10ZnO$+$7Na_2O$+x-α$Fe_2O_3$ where x=0, 0.1, 0.3, 0.6 mol% was investigated. XRD confirmed that the prepared glass series were non-crystalline. Fundamental physical characteristics including density, molar volume and related parameters were also calculated. The glass's density ranged from 2.73 to 2.76 $g/cm^3$ with increasing α-$Fe_2O_3$ content, while molar volume showed an opposite trend. UV-Visible spectroscopy was employed to analyse the optical behavior, showing a notable reduction in the optical bandgap from 3.24 to 2.76 eV. Overall, the findings suggest that the prepared glass materials hold strong potential for use in photonic applications.

**g0033**

**Impact of Zirconium Oxide on Physical, Structural, and Optical Properties of Lithium Boro-tellurite Glasses Ranjitha K N[1], Devaraja C[1, a)] and Ambika M R[2]**

[1]*Department of Physics, Manipal Institute of Technology Bengaluru, Manipal Academy of Higher Education, Manipal, India*
[2]*Department of Physics, M S Ramaiah Institute of Technology, MSR Nagar, Bengaluru 560054, India*
[a)] *Corresponding author. devaraja.c@manipal.edu*

Five glass samples with a specified composition of $65B_2O_3$-$15TeO_2$-X$ZrO_2$-$5Na_2O$-$10Li_2O$ (where X=0,0.2,0.4,0.6, and 0.8 mol%) are produced through the melt quenching method. The XRD confirmed that the samples were non-crystalline. The FTIR spectra of

BTNLZr glasses were verified and analyzed between 400-4000 $cm^{-1}$. The molar volume and density were evaluated. UV-visible spectroscopy was used to investigate optical absorption in the range of 200-800 nm. Optical characteristics, such as the Urbach energy and energy band gap, were calculated using specific methods. Absorption edge analysis has been used to evaluate the optical bandgap values. The range of the band gap values is 3.14 to 3.21 eV(direct) and 2.90 to 3.05 eV(indirect), respectively. According to the optical analysis, these types of glasses are used in optoelectronics and nonlinear optics applications.

**g0034**

**Design of a High Performance Flexible Mechanical Energy Harvester Based on Graphene Doped $Y_2O_3$-P(VDF-HFP) Nanocomposite**

Priti Sundar Barman, Prakriti Adhikary[a)]
*Department of Physics, University of North Bengal, Raja Rammohunpur, District: Darjeeling-734013, West Bengal, India*
*[a)] Corresponding author's E-mail: prakriti@nbu.ac.in*

Flexible piezoelectric nanogenerator $(PNG)$ fabricated by $Yttrium\ oxide\ (Y_2O_3)$, and $Graphene\ nanoplatelet$ doped composite film shows an maximum open circuit voltage output of $12\ V$. The capacitor-charging capability by the $PNG$ indicates its suitability for effectively harvesting mechanical energy from finger impact (a pressure amplitude of $\sim 11\ kPa$) and as an alternative in the area of self-powered energy harvesting devices.

**g0036**

**Exploring the Influence of Lanthanum doping on Electrical Properties of $K_{0.5}Bi_{0.5}TiO_3$ Ceramics**

Saloni Bhardwaj[1,a)], Shammi Kumar[2] and Nagesh Thakur[3]
*[1]Department of Physics, Ramjas College, University of Delhi, New Delhi-110009, India*
*[2]Department of Physics, Govt. College Nadaun Distt.- Hamirpur-177033, HP, India*
*[3]Department of Physics, Himachal Pradesh University, Shimla-171005, HP, India*
*[a]saloni.physics92@gmail.com (Email of corresponding author)*

Potassium bismuth titanate (KBT) of perovskite structure is among the lead-free piezoelectric and ferroelectric materials that promises a number of applications in sensors, Micro-electro-mechanical systems and actuators. However, KBT with rare earth doping has not been properly investigated, although KBT in bulk ceramic form has been widely studied. In this article, we synthesized lanthanum doped $K_{0.5}(Bi_{1-x}La_x)_{0.5}TiO_3$ at x = 0.0 and 0.3 by sol-gel technique. An optimized concentration has been taken to study the electrical and ferroelectric properties of lanthanum doped KBT. Leakage current density with electric field was observed from 20-200 $^oC$. According to current density electric field characteristics (J-E curve), ohmic conduction was determined to be the predominant conduction mechanism. The lanthanum doped ceramic exhibits low dielectric loss compared to the undoped KBT ceramic at room temperature. P-E loop traces demonstrated good saturation in the curves.

**g0037**

**Physical, Structural, and Optical Properties of Tellurium Soda-Borate Glasses Doped with Cerium Oxide**

Shivakumar B N[1] Vinay D[1] and Devaraja C[1,*]
*[1]Department of Physics, Manipal Institute of Technology Bengaluru, Manipal Academy of Higher Education, Manipal 576104, Karnataka, India*
**Email: devaraja.c@manipal.edu)*

This investigation is to explore how $CeO_2$ affects the physical, structural, and optical characteristics of tellurium soda-borate glasses. The conventional melt quenching technique was used to produce these novel glasses by adding different amounts of $CeO_2$ to the components of the tellurium soda-borate glasses. The non-crystalline nature of the samples was found by the XRD. The density of glass samples was determined by Archimedes' principle, and hence other physical properties were calculated. The optical properties were analyzed for the glass samples by the UV-Visible spectroscopy method. The direct energy band gap, indirect energy band gap, refractive index, and numerical aperture of the BTNC glasses were inclined by the variation of $CeO_2$ content. The highest refractive index (RI) value was reported for BTNC5. When $CeO_2$ was increased, the values of density, polaron radius, and oxygen packing density decreased. The results obtained indicate that the BTNC glasses are potential candidates for optical material applications.

**g0038**

**Effect of Sr in BST for Energy Applications**

Nibedan Nanda[1], Aman Malasi[1] and Pawan Kumar[1,*]
*Department of Physics and Astronomy, National Institute of Technology Rourkela, Odisha 769008, INDIA*
**Email: pawankumar@nitrkl.ac.in*

Lead-free $Ba_{1-x}Sr_xTiO_3$ (BST) ceramics with x = 0.25, 0.30, and 0.35 were synthesized via solid-state reaction for energy storage applications. X-ray diffraction confirmed the formation of a tetragonal phase. Among the compositions, 35BST exhibited superior dielectric and energy storage performance near room temperature, delivering a recoverable energy density of 0.75 $J/cm^3$ and efficiency of ~ 72.2 % at 115 kV/cm. Enhanced Sr content was found to improve breakdown strength and polarization, making BST a promising lead-free candidate for energy storage devices.

**g0039**

**Comparative Analysis of High Energy Ball Milling and Hand Grinding of Calcium Doped Barium Titanate Ceramics**

Susmita Garnayak[1], Sumit Kumar Giri[1], Pawan Kumar[1, *]
*[1] Department of Physics and Astronomy, National Institute of Technology Rourkela, Odisha, 769008, India*
*Corresponding author: E-mail ID: * pawankumar@nitrkl.ac.in*

The synthesis, structural characteristics, and functional properties of calcium-modified barium titanate ($Ba_{1-x}Ca_xTiO_3$) ceramics of composition x = 0.10 and 0.20 are studied. Two synthesis methods, high-energy ball milling (HEBM) and hand grinding (HG), are adopted to compare their impact on the material's ferroelectric, dielectric, and structural properties. XRD analysis confirmed the tetragonal perovskite structure for both ceramics. Density measurements revealed that HEBM samples have higher densities due to finer particle sizes and better sintering efficacy. FESEM further supported these results, showing that HEBM samples produced smaller, more uniform particles compared to the larger and less homogeneous particles from HG. Ferroelectric hysteresis loop measurements and room temperature dielectric study showed better ferroelectric properties and high dielectric constant for the HEBM sample, respectively, particularly for $Ba_{0.90}Ca_{0.10}TiO_3$.

**g0041**

**Evolution Of Microstructure, Dielectric And Magnetodielectric Properties Of LTNO With Mn Doping**

Srishti Kashyap and Sudip Mukherjee
*UGC DAE Consortium for Scientific research, BARC Campus, Trombay, Mumbai-400085, India*
**Email: ksrishti595@gmail.com, sudipm@csr.res.in*

2.0 mol% Mn substitution at Ni-site in high-k Li,Ti based NiO (LTNO) (henceforth called LTM-NO) has been accomplished by solid-state synthesis route to evaluate the microstructural, magnetic, dielectric and magnetodielectric behavior. Crystallographic structure and phase purity of sample is characterized by X-Ray Diffraction. Here, comprehensive investigation of pure cubic LTM-NO sample by magnetic measurements and temperature dependent dielectric spectroscopy are provided. The dc-magnetic properties manifest with pronounced several magnetic transitions in LTM-NO ($Li_{x=0.30}$, $Mn_{z=0.02}$) which are associated with the ferrimagnetic and antiferromagnetic orderings. Impedance spectroscopy measurements over a wide temperature range can be perfectly described with appropriate microstructural model, based on domain and domain boundary model, justifying the enhancement of the dielectric response of LTM-NO. Magnetodielectric study performed under fields upto 10 T reveals Mn-substitution reverses the negative magnetodielectric effect which was prevalent in LTNO.

**g0042**

**Positron Annihilation Lifetime Studies on Defect Structures in $LaAlO_3$ Perovskite and Their Correlation with Optical and Electronic Properties**

Ayush Sharma[1, 2], Shania D'souza[3], Nimai Pathak[1, 2, *], Dhanadeep Dutta[1, 2, *]
*[1]Radiochemistry Division, Bhabha Atomic Research Centre, Trombay, Mumbai-400 085*
*[2]Homi Bhabha National Institute, Anushaktinagar, Mumbai-400 094*
*[3]Institute of Chemical Technology, Mumbai-400 019*
*[*]Corresponding author: nimai@barc.gov.in, deep@barc.gov.in*

Defects in lanthanum aluminate ($LaAlO_3$), a perovskite-type oxide, play a critical role in modulating its structural, optical, and electronic properties, yet their characterization and control remain a significant challenge. In this study, $LaAlO_3$ was synthesized using a solid-state and molten salt-assisted co-precipitation methods, and the nature of intrinsic defects was investigated using Positron Annihilation Lifetime Spectroscopy (PALS). X-ray diffraction (XRD) and Fourier-transform infrared (FTIR) spectroscopy confirmed the formation of a single-phase rhombohedral perovskite structure in both the synthesis methods. PALS measurements revealed the variation in vacancy-type and large open-volume defects in the $LaAlO_3$ synthesized through two different routes. The variation in DC conductivity, evaluated through Broadband Dielectric Spectroscopy (BDS), indicated that these defects actively contribute to charge transport processes. Photoluminescence (PL) spectroscopy further revealed defect-related emission features, underscoring the potential of $LaAlO_3$ as a luminescent host material. The integrated structural, optical, and electrical characterizations establish $LaAlO_3$ as a versatile material with promising applications in phosphor technologies and dielectric devices.

**g0043**

**Enhancing Dielectric and Energy Storage Properties of PVDF-HFP Electrospun Fibers through Variation in Drum Collector Rotation Speed**

Sudhanshu Dhumrash and Poonam Uniyal[a)]
*Smart Material Laboratory, Department of Physics & Material Science, Thapar Institute of Engineering & Technology, Patiala, Punjab – 147004, India*
*[a)] Corresponding author: poonam.uniyal@thapar.edu*

PVDF-HFP thick films have been prepared by electrospinning technique and the effect of rotation speed (200 rpm, 500 rpm, 500 rpm) of drum collector has been studied on the structural, dielectric and energy storage properties. A systematic enhancement in the dielectric, ferroelectric and energy storage properties has been observed with an increase in the rotation speed. The fiber films prepared at 500 rpm i.e. (HP-500) possesses the highest discharged energy density of 2.53 J/cm3 and the highest value of dielectric constant i.e., 13.7.

**g0046**

**Effect of annealing temperatures on structural and dielectric properties of PVDF-5 KNN polymer –ceramic nanocomposite**

Ajeet Kumar, Poonam Uniyal[a)]

*Smart Materials Laboratory, Department of Physics & Materials Science, Thapar Institute of Engineering & Technology, Patiala, Punjab – 147004, India*

[a)] *Corresponding author: poonam.uniyal@thapar.edu*

A poly (vinylidene fluoride) (PVDF) – Sodium potassium niobate (KNN) nanorods-based PVDF – 5 KNN nanocomposite has been prepared using the solution casting method. The dispersion of KNN nanorods within the PVDF matrix leads to enhancing the electroactive phase (β-phase) with annealing temperature as estimated from X–ray diffraction. The dielectric constant increases with the addition of KNN nanorods in the PVDF matrix and is found to be highest for the film annealed at 80 ℃.

**g0047**

**Facile Fabrication of Flexible ZnO Nanorod-Based Tactile Sensors for Wearable Applications**

Laishram Anamika Devi[1], Prasanna Kumar S Mural[2], and Pramod Kumar[3,*]

[1]*Center for Research in Nanotechnology and Science (CRNTS), Indian Institute of Technology Bombay, Mumbai 400076, India*

[2] *Department of Metallurgical Engineering & Materials Science, Indian Institute of Technology Bombay, Mumbai 400076, India*

[3]*Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India*

[*]*Corresponding author: pramod_k@iitb.ac.in*

The development of flexible and low-cost tactile sensors is crucial for wearable electronics and electronic skin technology. In this study, we report a cost-effective and scalable flexible tactile sensor based on a facile seedless hydrothermal growth method for synthesizing zinc oxide (ZnO) nanorods (NRs) on flexible Indium Tin Oxide coated Polyethylene Terephthalate (ITO-coated PET) substrates. Unlike conventional approaches, the synthesis was carried out without any seed layer deposition, thereby reducing the fabrication complexity and cost. Structural and morphological analyses were performed using SEM and XRD, which confirmed the formation of densely packed, vertically aligned ZnO NRs on the substrate. The fabricated sensor demonstrated a low-pressure detection range of 0.33–1.33 kPa, corresponding to gentle touch stimuli, such as fingertip contact or light surface tapping. This study not only simplifies the device fabrication process but also demonstrates the potential of seedless ZnO NRs for tactile sensing applications, including artificial skin, soft robotics, and health-monitoring wearable devices.

**g0048**

**Dielectric and Vibrational studies of Compositionally Engineered Lead-Free NBT-Based Ferroelectric Materials**

V B Jayakrishnan[1a)], S K Mishra[1,3], Swayam Kesari[1], Rekha Rao[1,3], Suhas Phapale[2] and P U Sastry[1,3]

[1] *Solid State Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai, 400085, India*

[2]*Chemistry Division, Bhabha Atomic Research Centre, Trombay, Mumbai, 400085, India*

[3] *Homi Bhabha National Institute, Anushakti Nagar, Mumbai, 400094, India*

**Email: jayakris@barc.gov.in (Email of corresponding author)*

Lead-based materials are known for their toxicity and environmental concerns, driving research into Pb-free alternatives. Sodium bismuth titanate (NBT) shows high polarization and transition temperature, with potential in energy storage and many other applications. We studied modified NBT solid solutions with $NaNbO_3$ (xNBT) to induce inter-ferroelectric instabilities and morphotropic phase boundaries near room temperature using dielectric and Raman studies. Our x-ray/neutron diffraction results showcased the compositional phase transitions: $Pbma/Pmc2_1$ ($x<0.15$), Pbnm (0.15–0.20), Pbnm+P4bm (0.20–0.60), P4bm+R3c (0.60–0.80), and R3c ($x>0.80$). In this study the behaviour of dielectric constant and vibrational modes by Raman spectroscopy for various compositions and these results are correlated to structural changes.

**g0049**

**Development of Water Engineered Porous Conductive PDMS Composite for Piezoresistive Applications**

K. Varshney[1], S. P. Simma[2], R. K. Mondal[1], K. A. Dubey[1, a)], Y. K. Bhardwaj[1],

[1]*Radiation Technology Development Division, Bhabha Atomic Research Centre, Mumbai, India*

[2]*National Institute of Technology Surathkal, Karnataka, India*

**Email: abhinav@barc.gov.in*

Piezoresistive polymeric materials are gaining significant importance in present-day applications due to their lightweight, flexible, and wearable nature. They enable the development of advanced sensors for healthcare monitoring, soft robotics, and smart textiles. Their tunable mechanical-electrical response makes them ideal for next-generation energy harvesting and pressure-sensing devices. This study shows the synthesis of porous conducting PDMS/CCB composites and its rate dependent Piezoresistive behaviour. This work establishes critical design guidelines for rate-dependent Piezoresistive materials, providing a foundation for developing high-performance flexible pressure sensors with tailored dynamic response characteristics for advanced tactile sensing systems.

**g0050**

**Enhanced Dielectric Response in PVDF-$CoFe_2O_4$ Nanocomposite Thick Films**

Lovepreet Kaur Dhugga and Dwijendra P. Singh[*]

*Department of physics and materials science, Thapar Institute of Engineering & Technology, Patiala, Punjab-147004*

**Email: dpsingh@thapar.edu*

The fabrication of polyvinylidene fluoride (PVDF)-based thick films embedded with cobalt ferrite ($CoFe_2O_4$) nanoparticles has been considered to achieve superior dielectric performance. $CoFe_2O_4$ nanoparticles are uniformly incorporated into the PVDF matrix using a solution casting technique at varying weight fractions 20%-100% in the step size of 20wt.% and denoted as PC20, PC40, PC60, PC80 and PC100 with the thickness 0.05mm. The resulting nanocomposites are extensively characterized using X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), Fourier-transform infrared spectroscopy (FTIR), and impedance spectroscopy. Structural analysis confirmed the formation of the electroactive β-phase in PVDF. PC40 has achieved highest values for permittivity as $\varepsilon_r \sim 54.5$ with real (ε') and imaginary (ε") parts be ~ 54.3 and 5 respectively, along with low less ~ 0.09 at 1kHz. These findings underscore the influence of nanoparticle loading on tuning the dielectric behavior of PVDF-$CoFe_2O_4$ nanocomposites, positioning them as promising materials for applications in capacitors, sensors, microwave and energy storage devices.

**g0051**

**Cu-Substituted $YCrO_3$: Structural and Electrical Modifications for High-Frequency Devices**

Prachi Jain[1,2*], Mayank Goyal[2], O. P. Thakur[2]

[1] *Department of Physics, Vellore Institute of Technology, Amaravati, Andhra Pradesh-522241, India*

[2]*Materials Analysis and Research Laboratory, Netaji Subhas University of Technology, Sector-3, Dwarka, New Delhi-110078, India*

[*] *Corresponding author: prachi.jain@vitap.ac.in*

The current study comprises the extensive investigations on the structural, morphological, and electrical properties of the copper (Cu) substituted yttrium chromite nanoparticles [$YCr_{1-x}Cu_xO_3$ (x = 0.00, 0.05, 0.10)] prepared via modified sol-gel auto combustion synthesis route. The obtained HRXRD patterns confirmed the formation of orthorhombic structure with Pnma space group. The average particle size of the prepared samples has been calculated using FESEM studies. Whereas, the EDX studies confirmed the existence of elements present in the sample along with their % composition. The performed dielectric studies displayed the existence of conventional Maxwell-Wagner Polarization in all samples. The presence of the grain boundary contribution to the sample's relaxation is evident from the complicated impedance plot. The composition, x = 0.05, depicted maximum dielectric permittivity with low tangent loss, and very least value of impedance. Hence, these obtained results declare that the 5% Cu doped $YCrO_3$ (x = 0.05) is well suited for its development in high frequency devices applications.

**g0052**

**Morphotropic Phase Boundary Assisted Energy Storage Response in BCST Ceramics for Next Generation Green Energy Solutions**

Sachin Sharma[1, a)] Sanjeev Kumar[2] and N.S. Negi[1]

[1] *Department of Physics, Himachal Pradesh University, Summer Hill, Shimla, India, 171005*

[2] *Physics Department, Punjab Engineering College (Deemed to be University), Chandigarh, India, 160012*

*Corresponding author: risiani851@gmail.com*

The development of lead-free dielectric capacitors with high energy density is essential for next-generation green energy storage devices. However, balancing the trade-off between energy density and efficiency is a long-standing challenge for the realization of miniaturized pulsed power technologies. In this context, we developed $(Ba_{0.95}Ca_{0.05})(Ti_{0.93}Sn_{0.07})O_3$ ceramics using the sol-gel chemical route. The morphotropic phase boundary evolution is confirmed from Rietveld refinement of the XRD pattern. The presence of dielectric anomalies supports the tetragonal and orthorhombic phase coexistence in BCST ceramics. The BCST sample exhibits $W_{rec} \sim 155$ mJ/cm$^3$ and $W_{tot} \sim 217$ mJ/cm$^3$ with a corresponding efficiency of 72 % at a maximum applied electric field of 55 kV/cm with considerable frequency stability. These findings highlight Sn-induced MPB evolution and relaxor behavior as key factors that position BCST ceramics as a strong candidate for pulsed power and next-generation energy storage applications.

**g0053**

**Tailoring the Structure and Dielectric Behaviour of $BiFeO_3$ Nanoparticles via $La^{3+}$ A-Site Substitution**

Krina Ramani[1], Hetal Gohil[1], H.K. Rathod[1], Payal Joshi[1], D.K. Chudasama[2], V.G. Shrimali[2], P.S. Solanki[1], A.D. Joshi[3], Davit Dhruv[1], N.A. Shah[1, *)]

[1]*Department of Physics, Saurashtra University, Rajkot, 360005, Gujarat, India*

[2]*Government Polytechnic, Rajkot, 360005, Gujarat, India*

[3]*Department of Nanoscience and Advanced Materials, Saurashtra University, Rajkot, 360005, Gujarat, India*

**Email: snikesh@yahoo.com*

Bismuth ferrite (BFO) and lanthanum-doped bismuth ferrite (BLFO) nanoparticles have garnered significant attention due to their promising multiferroic properties and potential applications in spintronics, photocatalysis, and energy devices. The present study focuses on $BiFeO_3$ (BFO) and La-doped $BiFeO_3$ (BLFO) nanoparticles synthesized using the sol-gel method to investigate the impact of lanthanum substitution on their structural, morphological, and dielectric properties. X-ray diffraction (XRD) patterns revealed the creation of a perovskite structure with rhombohedral symmetry in BFO, which subsequently converted into an orthorhombic phase after La doping, showing structural distortion due to ionic substitution. Field Emission Scanning Electron Microscopy (FESEM) research found that grain size decreases as La content increases. Room temperature dielectric studies showed a drop in dielectric constant as La concentration increased, which might be attributed to reduced space charge polarization and oxygen vacancy suppression. Temperature-dependent dielectric studies (from room temperature to 400 °C) revealed increased

thermal stability and dielectric constant with higher temperatures. The results demonstrate that La doping via the sol-gel technique is a viable strategy to tune the microstructure and dielectric behaviour of BFO ceramics for possible applications in multifunctional electrical and energy devices.

**g0054**

**Filler Dependent Enhanced Dielectric Performance in PVDF/KNN Composites: Broadband Frequency Analysis in Relation to Microstructural Correlations**

Satyam Dubey[1], Maheswar Panda[1,*] and Dinesh Kumar Shukla[2]
[1]*Multifunctional Polymer Nanocomposites Laboratory, Department of Physics, Dr. Harisingh Gour Vishwavidyalaya (A Central University), Sagar, M.P.- 470003, India*
[2]*UGC-DAE Consortium for Scientific Research, University Campus, Indore, M.P.-452001*
**Email: mpanda@dhsgsu.edu.in*

In this study, the cold-pressed polymer nanocomposites (PNC) of PVDF and K0.5Na0.5NbO3 (prepared through the Hydrothermal method) were prepared with the help of a hydraulic press at room temperature under 20MPa in varying wt% (10,20,30,50,60). The PNC was characterized for structural, micro-structural, & Dielectric properties respectively. X-ray diffraction confirmed phase-pure KNN formation, while FESEM revealed micro-sized particles (2-11 μm) and nanorod morphologies with good dispersion in the PVDF matrix. Dielectric spectroscopy (10 Hz to 1 MHz) demonstrated significant enhancement in dielectric constant from $\varepsilon_r \approx 12$ for pure PVDF to $\varepsilon_r \approx 88$ for 60 wt% KNN composites, while maintaining relatively low loss tangent ($\tan\delta < 0.3$). The composites exhibit stable, frequency-independent dielectric behavior, demonstrating their potential for room-temperature ferroelectric and dielectric applications.

**g0055**

**Influence of Large Grain Size on $Ba(Zr_{0.20}Ti_{0.80})O_3$-0.48$(Ba_{0.70}Ca_{0.30})TiO_3$ Piezoelectric Ceramic**

Priyanka Sharma[1], Meena Devi[1], Komal Arora[1], Sanjeev Kumar [2], Rajat Syal[3]
[1] *Department of Applied Sciences, Chandigarh Group of Colleges, Landran, Mohali, Punjab - 140307, India*
[2] *Department of Physics, Punjab Engineering College (Deemed to be University), Chandigarh - 160012, India*
[3] *Department of Physics & Photonics Science, National Institute of Technology, Hamirpur, H.P. -177005, India*
[1]*Corresponding author: rajatsyal1994@gmail.com*

We have performed systematic investigation on $Ba(Zr_{0.20}Ti_{0.80})O_3$-0.48$(Ba_{0.70}Ca_{0.30})TiO_3$ composite fabricated using traditional solid-state method, and their physical properties were systematically examined. The ceramics have been studied for structural, morphological, ferroelectric, dielectric, and ferroelectric characteristics. XRD results revealed that the ceramic shows the pure perovskite structure, and the large grain size ~ 23.05μm has been observed in the prepared composition. Ceramic exhibits the large value of room temperature dielectric constant ~ 3247 and low dielectric loss ~ 0.04. The saturated ferroelectric loop behaviour in polarization vs electric field curve has been observed in the ceramic. The observed values of remnant polarization ($P_R$), saturation polarization ($P_S$) and low values of coercive field ($E_C$) are 11.4 μC/cm$^2$, 21.4 μC/cm$^2$ and 2.15 kV/cm, respectively. The ceramic possesses excellent piezoelectricity, with $d_{33}$ ~ 414 pC/N and $K_P$ ~ 52.5% showing that it has great piezoelectric characteristics.

**g0056**

**Comparative Study of Structural, Microstructural, Dielectric, and Energy Storage Properties of $Bi_{0.5}Na_{0.5}TiO_3$ and $SrTiO_3$-doped $Bi_{0.5}Na_{0.5}TiO_3$ Ceramic**

Amiya Mandal[1,*] and Kanhaiya Lal Yadav[1, 2]
[1]*Smart Material Research Laboratory, Department of Physics, Indian Institute of Technology Roorkee, Roorkee 247667, India*
[2]*Centre for Sustainable Energy, Indian Institute of Technology Roorkee, Roorkee 247667, India*
**Email: amiya_m@ph.iitr.ac.in*

In this study, we investigated the outcome of $SrTiO_3$ (ST) doping on the performance of energy storage of $Bi_{0.5}Na_{0.5}TiO_3$ (BNT)-based ceramics. A 0.8BNT–0.2ST composition was synthesized via the conventional solid-state route and characterized for structural, microstructural, and dielectric properties. X-ray diffraction confirmed the formation of a single-phase P4bm perovskite structure, and FESEM analyses showed a noticeable reduction in grain size with 20wt% ST doping. A reduction in the dielectric constant was observed, along with a downward shift in the phase transition temperature. Consequently, an obvious improvement in recoverable energy density ($W_{rec}$) and efficiency ($\eta$) had been noticed from ferroelectric results, reflecting enhanced relaxor characteristics in the doped specimen. Overall, $SrTiO_3$ addition was found to be an effective strategy for boosting the energy storage capability of BNT ceramics.

**g0057**

**Structural, Magnetic, Electrical and EMI Shielding Properties of Iron Oxide Impregnated Coconut Shell Charcoal**

Prof. Deepa Seetharaman
*Department of Physics, Sri Sathya Sai Institute of Higher Learning, Anantapur Campus, 515001*
**deepaseetharaman@sssihl.edu.in*

Eco-friendly procedure of natural soaking was adopted to synthesize iron oxide impregnated coconut shell charcoal powder. The as-synthesized product was calcined further at high temperature to improve its magnetic properties. Thick sheets of PVDF composites were prepared using these calcined powders as filler. Electrical studies showed that the dielectric constant showed 10-

fold and the electrical conductivity showed 1000-fold enhancement compared to pristine PVDF. A maximum total EMI shielding effectiveness of 24 dB was achieved along with ~ 34% absorption for a 1.4 mm thick polymer composite sheet showing the potential of this composite for microwave absorption applications.

**g0058**

**The Influence of La doping on Ceria for the Enhancement of Dielectric Properties**

Anshu Singh[1]*, Akanksha Malik[1], Richa Saini[1], Pawan kumar[2], Asokan Kandasami[3]
[1]*Department of Physics, Kanya Gurukul Campus, Gurukul Kangri (Deemed to be University), Haridwar, Uttrakhand-249404, India*
[2]*Department of Physics, Government College for Women, Bawani Khera, Haryana – 127032, India*
[3]*Department of Physics & Centre for Interdisciplinary Research, University of Petroleum and Energy Studies (UPES), Dehradun, Uttarakhand-248007, India.*
*Email: anshu.singh2105@gmail.com**

Ceria (CeO2) nanoparticles were prepared using sol-gel method. X-ray diffraction (XRD), scanning electron microscopy (SEM), resistivity vs temperature (R-T) and dielectric measurements were employed to characterize the samples. XRD analysis confirmed the formation of FCC structure corresponding to CeO2 with space group Fm3m. SEM investigations revealed that the CeO2 nanoparticles with an average particle size of ~15.64 nm. The resistivity of samples was found to be enhanced with La concentration in CeO2. Furthermore, the dielectric measurements were performed as a function of frequency at room temperature as well as temperature shows an enhancement in dielectric constant with La doping.

**g0059**

**Structural, Dielectric and Optical Properties of $Ba_{0.97}Tb_{0.03}TiO_3$ perovskite Ceramic**

Sadhana Yadav[, 1)] and Akhilesh Kumar Singh[1, a)]
[1]*School of Materials Science and Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi-221005, India*
[a)] *Corresponding author: aksingh.mst@iitbhu.ac.in*

In this work, we have investigated the effects of $Tb^{3+}$ ion on structural, dielectric and optical properties in $Ba_{1-x}Tb_xTiO_3$ (i.e. x = 0.03 mol) perovskite ceramic synthesized through high energy ball milling method. The structural analysis of the X-ray diffraction (XRD) data reveals the tetragonal phase with P4mm space group. The average grain size of the $Ba_{0.97}Tb_{0.03}TiO_3$ was calculated using HR-SEM image and found to be 0.629 µm. The temperature dependent dielectric study reveals the maximum relative dielectric permittivity($\varepsilon_r$)~4700 at 10 kHz with low loss less than 1. The diffuse reflectance spectroscopic spectra contain a broad band at 355 nm along with a peak at 681 nm due to 4f-4f transition of $Tb^{3+}$ ions. The optical band gap of $Ba_{0.97}Tb_{0.03}TiO_3$ was calculated by using the diffuse reflectance spectroscopic spectra and found to be 3.28 eV. These characteristics of synthesized materials may be useful for potential application in capacitive energy storage and LEDs.

**g0060**

**Dielectric loss of $Gd^{2+}$ doped lead titanate fabricated by high energy ball milling method**

Sona Kumari[1,] Sweta Sinha[2] and R. K. Chaudhary[3]
[1]*Assistant Professor, RTC Institute of Technology, Anandi Ormanjhi, Ranchi, Jharkhand, India*
[2]*Assistant Professor, Amity University, Ranchi Jharkhand*
[3]*Ex Professor and Head, NIT Jamshedpur, Jharkhand, India*
*Corresponding author: a) sona_kumari@rtcit.ac.in, [b)] sonakumariphy@gmail.com*

Our presumption is that this modification will be more dependent on the ionic radii difference. Such type of studies has hardly been reported as such lead titanate having perovskite structure ($ABO_3$) has been selected as host lattice gadolinium as the source of guest ions. Ceramic powder has been fabricated by using High Energy Ball Milling (HEBM) method, keeping these things in mind fabrication has been done in a systematic way. Dielectric constant is minimum for undoped lead titanate sample and increases by about five percent (5%) for gadolinium doped samples. It also appears from the figures that for five percent (5%) gadolinium samples Tc shift to higher temperature side.

**Keywords**: Dielectric constant, Curie Temperature, high energy ball milling, lead titanate, and dielectric loss etc.

**g0061**

**Mechanical Energy Harvesting by Quantum Rod Incorporated with Poly (vinylidene fluoride) Nanogenerators**

Srishti Mridha[1], Abiral Tamang[1, *]
[1]*Department of Physics, Jadavpur University, Kolkata 700032, India*
** Email: abiralt.physics@jadavpuruniversity.in*

In this work, cadmium selenide (CdSe) core quantum rods (QRs) induced electroactive phase nucleation in poly (vinylidene fluoride) (PVDF) free standing films has been investigated. The prepared QR-PVDF composite (PQRF) films show higher electroactive content ($F_{EA}$ ~ 75%) than that of pure PVDF films, resulting in a better voltage output ($V_{OC}$ ~ 18V) coming from nanogenerator (NG) fabricated from PQRF films than that of NG made with PVDF film, under similar pressure application. The flexibility of PQRF nanogenerator makes it suitable for wearable sensors for physiological motion detection. As CdSe QRs have unique optical properties like highly polar photoluminescent emission at tunable wavelength, the PQRF composites could pave their way into the field of optoelectronic flexible nanogenerators.

**g0062**

**Structural, Morphological and Dielectric Characteristics of Gamma-Irradiated $CeO_2$-$TiO_2$ Nanocomposites**

Charul Uniyal[1,a)], Manoj Yadav[1], Ankur Kumar[2], Anshu Singh[3], Akanksha Malik[3], R.C. Meena[4]

[1]*Department of Physics, Sri Dev Suman Uttarakhand University Campus Rishikesh, Uttarakhand- 249201, India*

[2]*Department of Physics, Sri Dev Suman Uttarakhand University Campus Gopeshwar, Uttarakhand-246401, India*

[3]*Department of Physics, Kanya Gurukul Campus, Gurukul Kangri Deemed to be University, Haridwar, Uttarakhand-249404, India*

[4]*Materials Science Division, Inter University Accelerator Centre, New Delhi-110067, India*

[a)] *Corresponding author: charuluniyal2@gmail.com*

This study investigates the effect of gamma irradiation on the structural, morphological, and dielectric properties of $CeO_2$-$TiO_2$ nanocomposites. The XRD spectra showed that gamma irradiation causes intensity reduction and peak broadening, which are signs of increased lattice strain and decreased crystallinity without phase change. FE-SEM imaging showed that irradiation causes notable morphological changes, including increased surface roughness, improved particle aggregation, and the development of defect-rich linked networks. Furthermore, the dielectric measurements were performed as a function of frequency at room temperature as well as temperature which shows an enhancement in dielectric constant with irradiation. The overall improvement in dielectric performance implies that $CeO_2$-$TiO_2$ nanocomposites can be effectively tailored using gamma irradiation for advanced high-k dielectric and capacitor applications.

# h) Transport properties and semiconductor physics

**h0001**

**Polar Resistors**

Aditya N. Roy Choudhury
*Independent Researcher, Kolkata, India*
**Email: roychoudhury.aditya.2021@gmail.com*

It is seen that semiconductor INI structures give polar resistance when the thicknesses of the I (intrinsic) layers are properly tuned. A polar resistor (or, a directional resistor) is a resistor that has two values of resistance – each for a direction of current. When the current direction through the resistor changes the resistance value also changes. In this work, simulations are done for 3 semiconductor INI structures (Si, Ge and GaAs) and it is seen that all 3 show polar resistance between -1 V and +1 V (for I layer thicknesses varied between 100 μm and 500 μm for Si, 5 μm and 20 μm for Ge, and 3000 μm and 10,000 μm for GaAs). The N layer doping density is kept at $10^{15}$ /cc. N-type, $10^{18}$ /cc doped CdS (electron affinity = 4.5 eV) for Si, CdTe (electron affinity = 4.3 eV) for Ge, and $SnO_2$ (electron affinity = 4.7 eV) for GaAs can act as ohmic contacts giving the semiconductor structures a NININ configuration. Polar resistors can be used to add amplitude asymmetry to electrical waveforms in signal processing and music technology.

**h0002**

**Mn-Tuned CdTe Polycrystals: A Versatile Material for Optoelectronics & Spintronics**

Staines Obed James Johnson[1], Rajesh Paulraj[1, a)]
*[1]Scintillaton Materials Laboratory Department of Physics, Sri Sivasubramaniya Nadar College of Engineering, Kalavakkam, Tamilnadu – 603 110, India.*
*[a)] Corresponding author: rajeshp@ssn.edu.in*

Polycrystalline $Cd_{1-x}Mn_xTe$ (x = 0.08, 0.12) samples were synthesized using an indigenously developed horizontal furnace Optical absorption studies in the UV–Vis–NIR range showed a low absorption coefficient (~0.17–0.20 $cm^{-1}$ at 980 nm), along with a systematic increase in bandgap energy with rising Mn concentration. Negative photoconductivity was also observed, indicating potential in infrared photodetectors and optical isolators. Room-temperature magnetic analysis revealed distinct ferromagnetic behavior, with both magnetization strength and hysteresis loop area increasing with Mn concentration.

**h0003**

**Fabrication and Characterization of Reactively rf Sputtered Titanium Oxide-Based Metal-Oxide-Semiconductor Devices**

Dip Manna[1, 2, a)], Koushik Mondal[1,2], Pawan Kumar Ojha[1], Prasanta Karmakar[3] and Supratic Chakraborty[1]
*[1]Saha Institute of Nuclear Physics, 1/AF, Bidhannagar, Kolkata-700064, India*
*[2]Homi Bhabha National Institute, BARC Training School Complex, Anushaktinagar, Mumbai-400094, India*
*[3]Variable Energy Cyclotron Center, 1/AF Bidhannagar, Kolkata 700 064, India*
**Corresponding author: mannadip1998@gmail.com*

This work investigates the resistive switching and dielectric properties of Ag/$TiO_x$/n-Si metal-oxide-semiconductor devices for potential applications in non-volatile memory and neuromorphic computing where $TiO_x$ film was deposited on Si substrates using reactive rf sputtering. X-ray photoelectron spectroscopy study indicates presence of $Ti^{4+}$ states and oxygen vacancies. Bipolar resistive switching behaviour is observed in the I-V characteristics with distinct set and reset voltages indicating reliable memory operation. Further, a non-volatile nature in the I–V data is also distinctly visible. C-V measurements reveal stable dielectric performance with minimal/no hysteresis suggesting low interface trap density. The combined results demonstrate that $TiO_x$-based devices offer promising performance for both memory and synaptic applications. Further, the suitability of Ag/$TiO_x$/n-Si structures is also evidenced for future memory device applications.

**h0004**

**Correlation of Structural and Optical Modifications in GaN Irradiated with Swift Heavy Ions**

Muskan Verma[1], Vinay Kumar[1], Dinakar Kanjilal[2], and Ashish Kumar[1*]
[1]*Department of Physics and Astronomical Sciences, Central University of Jammu, Rahya-Suchani, Samba J&K, India --181143*
[2]*Inter-University Accelerator Centre, Aruna Asaf Ali Marg, Vasant Kunj, New Delhi, Delhi, India–110067.*
**Corresponding author: dr.akmr@gmail.com, ashish.phy@cujammu.ac.in.*

GaN hold applications in space electronics, power devices, nuclear reactors, etc. However, these applications often operate in extreme radiation environments, which can degrade device performance or even cause failure [1,2]. Therefore, understanding the mechanisms behind radiation-induced degradation is crucial for enhancing device reliability and material applications in radiation rich conditions. GaN was irradiated using swift heavy Ni and Ag ions having 50 MeV and 200 MeV energy at a fluence of $1\times10^{10}$ ions/$cm^2$ at 300K. The effect of ion irradiation is studied through XRD, PL, and UV-Vis. spectroscopy. XRD studies revealed lattice disorder on irradiation resulting in induction of stress in the GaN layer. PL studies are consistent with the XRD studies, which indicated the creation of some deep-level defects in both the cases along with a high intensity near band emission ~3.43 eV, evident from UV-Vis. studies.

**h0005**

**Optical and Capacitive Properties of $Fe_2O_3$-$Sb_2O_3$ Composites for Multifunctional Sensing Applications**

Chetan Prakash Saini and A.P. Singh

*Department of Physics, Dr. B. R. Ambedkar National Institute of Technology, Jalandhar, Punjab, India*
**Email:jaiswarsinghap@nitj.ac.in*
The $Fe_2O_3$-$Sb_2O_3$ composite pellets were synthesized with varying $Sb_2O_3$ content to explore their multifunctional potential in sensing and electronic applications. The room temperature (RT) X-ray diffraction results confirmed pure and composite phases. UV-Vis spectroscopy revealed tunable band gaps, influenced by particle size and electronic structure modifications. Capacitance measurements across different frequencies showed enhanced dielectric response, particularly at 3 wt.% of $Sb_2O_3$. The frequency-dependent electrical behavior was strongly correlated with optimum concentration and defect-mediated charge dynamics. These composites exhibit promising properties for optical and capacitive sensing, enabling their potential use in multifunctional devices such as humidity and gas sensors. The study highlights their versatility as a platform for multifunctional device applications.

**h0006**

**Broken Inversion Symmetry Mediated Charge Order Fluctuations in Quasi 1D System $(NbSe_4)_3I$**

Soham Das[1], Mintu Mondal[1*]
*[1]School of Physical Sciences, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700032, India*
**Email: sspmm4@iacs.res.in (Email of corresponding author)*
We investigate resistance fluctuation across charge order disorder transitions in single crystal of $(NbSe_4)_3I$. We identify Charge order state and other possible symmetry reduced states through electrical and thermal transport measurement. The single crystal XRD analysis shows the non-centrosymmetric structure below charge order transition ($T_{CO}$ ~ 274 K). Electrical transport measurement indicates the activated behavior of resistivity followed by an enhancement of small gap at charge order transition which also confirmed by our band structure calculation using density functional theory. Additional symmetry lowered state is also verified through low frequency 1/f noise and Seebeck coefficient measurement near $T_d$ ~160K. We also find a strongly correlated phase at the temperature T* ~ 200 K coming from the enhancement of hole mobility within electron dominated thermal transport region. Our study delights a path for noise study on single crystal (NbSe4)3I with different symmetry and phonon interaction mechanism followed by presence of variable activated region with temperature. This work illustrates the effect of symmetry reduction in electrical and thermal transport.

**h0007**

**Room-Temperature Topological Phase Transition with Peierls Instability in a Quasi-one-dimensional $Bi_4I_4$**

Deep Singha Roy[1], Mintu Mondal[1, a)]
*[1]School of Physical Sciences, Indian Association for the Cultivation of Science, Jadavpur, Kolkata-700032*
*[a)] Corresponding author: sspmm4@iacs.res.in*
Higher-order topological insulators emerged as an extension to the traditionally existing domain of topological insulators with symmetry-protected states in edges or corners. Pristine $Bi_4I_4$ is a unique quasi-1-dimensional candidate with the simultaneous existence of edge/hinge modes [1]. We report resistance fluctuation dynamics at the very vicinity of room temperature topological phase transition from α-Bi4I4 (hinge modes) to β-Bi4I4 (surface states) mediated by the thermodynamically first-order structural transition inferred from differential Scanning Calorimetry. Inter-band transition is identified from the temperature-dependent Seebeck study Additionally, we identify a coexisting meta-stable phase from time-series resistance fluctuations and their inherent bi-modal distributions. This has been identified as Random Telegraphic Noise (RTN) [2,3]. This nature in the time domain resistance fluctuation is observed at around 306.8K, a bit prior to the phase transition that suggests a metastable phase persisting in the hysteretic domain of the resistivity curve.

**h0008**

**Electronic Structure And Transport Properties Of Kagome Semimetal $Co_{1-x}Mn_xSn$**

Rajesh Kumar Sahu[1, 2], Archna Sagdeo[1, 2], Rashmi Singh[3], Sanskar Mishra4, Prashant Shahi[4] and Soma Banik[1, 2]
*[1]Accelerator Physics and Synchrotron Utilization Division, Raja Ramanna Centre for Advanced Technology, Indore 452013, India*
*[2]Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400094, India*
*[3]Photonics Materials Technology Section, Raja Ramanna Centre for Advanced Technology, Indore 452013, India*
*[4]Deen Dayal Upadhyaya Gorakhpur University, Gorakhpur 273009, India*
** rajeshsahu@rrcat.gov.in (Email of corresponding author)*
Tailoring the properties of topologically protected flat bands and the Dirac point in 2D Kagome semimetal CoSn with doping promises more efficient and powerful device applications in spintronics and thermoelectricity. Here, we have performed a detailed study of the crystal structure, transport properties, and electronic structure of $Co_{1-x}Mn_xSn$ single crystals with $x = 0.01$ and 0.08. A systematic increase in lattice parameters and resistivity has been observed with increasing $x$. The value of the Seebeck coefficient becomes less negative for $x = 0.08$ compared to $x = 0.01$, indicating hole-like doping. Analysis of core levels revealed a decrease in spin-orbit splitting, an increase in peak broadening, and a shift of the peaks towards higher binding energy with increasing $x$. Valence band spectra showed that the feature corresponding to the flat band in Mn-doped compositions shifts towards the Fermi level as compared to CoSn. With an increase in $x$, the Dirac point as well as the bulk states are found to shift away from the Fermi level, which gives rise to an increase in the resistivity and the Seebeck coefficient in $Co_{1-x}Mn_xSn$.

**h0009**

**Development and Characterization of *p*-Type Transparent Conducting Oxides: A Study on Pure $CuGaO_2$ and $Ga_2O_3$-Modified $Cu_2O$ Compounds for Transparent Electronics**

Abhija D S[1], Chetan Prakash Saini[1], and A. P. Singh[1.a)]
[1]*Department of Physics, Dr. B. R. Ambedkar National Institute of Technology, Jalandhar, Punjab, India-144008*
**jaiswarsinghap@nitj.ac.in*

Transparent conducting oxides (TCOs) are critical for optoelectronic devices due to their unique combination of optical transparency and electrical conductivity. While *n*-type TCOs are well developed, efficient *p*-type TCOs remain a challenge. This study explores pure $CuGaO_2$ and $Ga_2O_3$ modified $Cu_2O$ (5 wt.% and 7 wt.%) as a potential *p*-type TCO material. Samples were synthesized via the conventional solid-state reaction route, and characterized for their structural, optical, and electronic properties using X-Ray Diffraction, UV-Visible spectroscopy, and Hall transport measurements. Structural analysis confirmed phase formation and crystallinity, while optical studies revealed direct band gaps and good transparency in the visible range. Hall measurements verified *p*-type conductivity, with $Ga_2O_3$ doping influencing carrier concentration and mobility. The findings suggest that both $CuGaO_2$ and $Ga_2O_3$:$Cu_2O$ systems are promising candidates for future *p*-type transparent electronics.

**h0010**

**An Emerging Class of Thermoelectric Materials: Vacancy-Ordered Double Perovskites $Cs_2NiF_6$ by DFT Study**

Deepali Shukla[1], Preeti Kumari[2], A. Shukla[1], and Ramesh Sharma[3,*)]
[1]*Department of Physics, University of Lucknow, Lucknow, (U.P) India*
[2] *Sri Chaitnya Technical Campus, Hyderabad, Telangana, India*
[3]*Department of Applied Science, Feroze Gandhi Institute of Engineering and Technology, Raebareli-229001, (U.P) India *Email: sharmadft@gmail.com*

The electronic structure, Seebeck coefficient, power factor, and thermoelectric figure of merit of the halide vacancy ordered double perovskite $Cs_2NiF_6$ are discussed inside the framework of density functional theory (DFT) using both PBE and mBJ functionals. According to electronic band structure calculation, it is found that the compound is an indirect band gap semiconductor with band gap equivalent to 1.69 eV (PBE-GGA) and 3.77 eV (TB-mBJ). Additionally, the constant relaxation time approximation is used in the semi-classical Boltzmann transport equations. The analysis shows that $Cs_2NiF_6$ has a high Seebeck coefficient of 3252.50 $\mu VK^{-1}$ for holes doping at 300 K. It is anticipated that this material has potential for useful energy conversion and storage devices because of the high Seebeck coefficient.

**h0011**

**Symmetry Analysis of Axion Insulating Phase in Magnetic Topological Heterostructures**

Juhi Singh[*] and Narayan Mohanta
*Department of Physics, Indian Institute of Technology Roorkee, Roorkee 247667, India*
**)juhi_s@ph.iitr.ac.in*

We investigate axion-insulating phases in magnetic topological heterostructures using slab models of $Bi_2Se_3$ and $MnBi_2Te_4$. In ferromagnet–topological insulator–ferromagnet (FM/TI/FM) trilayers, parallel spin alignment leads to quantized Hall conductivity due to broken time reversal symmetry (TRS), while antiparallel alignment yields a zero Hall plateau via effective TRS. $MnBi_2Te_4$ exhibits similar behavior: odd layers behave as Chern insulators and even layers as axion insulators. Our first-principles calculations confirm quantization of magnetoelectric coupling coefficient ($\theta \approx \pi$) for $Bi_2Se_3$. We highlight inversion symmetry and effective TRS as an essential ingredient for realizing axion phases.

**h0012**

**Effect of Site-Specific Substitution on Thermoelectric Properties of NiTiSn Based Half Heusler Alloys**

Yatin P. Desai and K. R. Priolkar [a)]
*School of Physical and Applied Sciences, Goa University, Taleigao Plateau, Goa 403206, India*
*[a)]Corresponding Author: krp@unigoa.ac.in*

Site-specific substitution in NiTiSn based Half-Heusler alloys ($NiTi_{0.95}V_{0.05}Sn$, $NiTiSn_{0.95}Sb_{0.05}$, $Ni_{0.95}Cu_{0.05}TiSn$) was examined using XRD, confirming the cubic C1b structure with near-stoichiometric compositions. Measurements of electrical resistivity, Seebeck coefficient, and power factor between 100–400 K showed that V-substitution at the Ti site achieved the highest PF (~25 mW $m^{-1}$ $K^{-2}$ at 400 K). In comparison, Sb and Cu substitutions led to marginal improvements, indicating Ti-site substitution as the effective strategy for enhancing thermoelectric performance.

**h0013**

**Synthesis and study of Optical and Electrical Properties of pure and doped Graphene Quantum Dots Thin Film**

Adesh Kumar[*] and Subhash Chand
*Department of Physics & Photonics Science, National Institute of Technology, Hamirpur, India, 177005 (HP)*
** Email: kumaradesh1000@gmail.com*

This study involves the synthesis and investigation of the optical and electrical properties of pure and doped graphene quantum dot thin films deposited on a quartz substrate, prepared using both hydrothermal synthesis and spin-coating methods. The UV-Visible study reveals a high absorption peak in the ultraviolet region, with a direct band gap of 4.51 eV, as calculated using Tauc's plot. It was observed that the prepared thin films show a high optical transmittance of 83% in the visible region at 500 nm. In addition to

this, the high temperature I-V characteristics have been studied in the temperature range of 393 K - 513 K. The calculated value of activation energy depicts the semiconducting behavior of the prepared graphene quantum dot thin films. It was found that the high optical transmittance and semiconducting nature of graphene quantum dot thin films show their applicability as a transparent conducting material in optoelectronic devices.

**h0014**

**Engineering Self-Powered Photovoltaic Response in Multi-Heterostructure p-$MoS_2$/n-$MoSe_2$ TMDC Devices via Series and Parallel Architectures**

Shreya Gaonkar[1, *], Manoj Kumar B[1], Rashed H. Lone[1,2], Agnibha Sarkar[1], E S Kannan[1]

[1]*Department of Physics, Birla Institute of Technology and Science, Pilani-K. K. Birla Goa Campus, Zuarinagar, Goa-403726, India.*

[2]*Functional Materials and Microsystems Research Group and the Micro Nano Research Facility, RMIT University, Melbourne, Victoria 3000, Australia.*

**Email:Shreyagaonkar35@gmail.com*

Two-dimensional transition metal dichalcogenide (TMDC)-based devices hold great promise for photovoltaic and optoelectronic applications. However, enhancing key performance parameters such as open-circuit voltage ($V_{OC}$) and short-circuit current ($I_{SC}$) remains a critical challenge. In this study, we systematically compare TMDC p–n junctions composed of Nb-doped $MoS_2$ and intrinsic $MoSe_2$ configured in both series and parallel arrangements with ITO electrodes. The series-connected device exhibits a $V_{OC}$ of approximately 0.5 V and an $I_{SC}$ of ~26 nA, with a rectification ratio of 10. In contrast, the parallel configuration yields a significantly higher $I_{SC}$ of ~170 nA, a $V_{OC}$ of ~0.3 V, and an enhanced rectification ratio of $10^3$. These results highlight the crucial role of device architecture in optimizing the photovoltaic response of TMDC heterojunctions.

**h0015**

**Investigation of the $D0_{22}$ Phase Stability and Magnetotransport Properties in $Mn_{2.9}Ga_{1.1}$ Alloy**

Sourav Mandal, Subrata Biswas, Harekrushna Behera, and Perumal Alagarsamy

*Indian Institute of Technology Guwahati, Guwahati-781039, Assam, India*

**souravmandal@iitg.ac.in*

$Mn_3Ga$ is a multifunctional Heusler-like compound that exists in several crystallographic phases, including hexagonal ($D0_{19}$), cubic ($L2_1$), and tetragonal ($D0_{22}$) structures, each exhibiting unique magnetic and electronic properties. Among these, the $D0_{22}$ phase has attracted significant interest for spintronic applications due to its combination of high uniaxial magnetocrystalline anisotropy and ferrimagnetic ordering. The $D0_{22}$ phase of $Mn_3Ga$ offers a rare balance of low saturation magnetization and high spin polarization, making it promising for spin-transfer torque magnetic random access memory devices. Moreover, its good electrical conductivity, coupled with large anomalous Hall effect and low Gilbert damping, enhances its potential for spintronic devices. In this study, $Mn_3Ga$ alloy was synthesized via arc melting and annealed to stabilize the tetragonal $D0_{22}$ phase. The structural, magnetic, and transport properties were systematically investigated. Remarkably, these properties remained largely unaffected by the choice of annealing medium, indicating the stability of the $D0_{22}$ phase under varying thermal conditions. Detailed results and analysis, focusing on its structural, magnetic, and transport characteristics of the prepared alloy, will be presented.

**h0016**

**Synergistic Role of Voltage in Tuning Resistive Switching Phenomenon of Sr2FeTiO6 Thin Films**

Richa Bharti[1a], Lipika Sasmal[1], Ranjan Kumar Malik[1], and Ajay D. Thakur[1]

*Department of physics, Indian Institute of Physics Patna, Bihta-801106, India*

*[a]Corresponding author: richa_2321ph11@iitp.ac.in*

We observe a reversible transition from volatile to non-volatile resistive switching in Ag/$Sr_2FeTiO_6$ (SFTO)/$SrRuO_3$ (SRO)/Si device upon applying higher voltage in the presence of a magnetic field. This behavior highlights the tunability of resistive switching under combined electric and magnetic stimuli and points toward the role of magnetoelectric coupling in complex oxides. The ability of the device to reversibly switch between volatile and non-volatile states makes it a strong candidate for use as a selector element in crossbar memory architectures. Furthermore, this switching characteristic opens new possibilities for developing multistate, high-density data storage in future memory technologies.

**h0017**

**Mn-Doped $Cs_2AgInCl_6$ Microcrystals For Lead-Free X-Ray Scintillation**

Aakash Singh[1], Mohit Tyagi[2], Santosh K. Gupta[3], Sai Santosh Kumar Raavi[1,4,a)]

[1] *Ultrafast Photophysics and Photonics Laboratory, Department of Physics, Indian Institute of Technology Hyderabad, Kandi 502285, Telangana, India.*

[2] *Technical Physics Division, Bhabha Atomic Research Centre, Mumbai, 400085 India.*

[3] *Radiochemistry Division, Bhabha Atomic Research Centre, Mumbai 400085, India; Homi Bhabha National Institute, Mumbai 400094, India.*

[4] *Department of Climate Change, Indian Institute of Technology, Hyderabad 502284, India*

*[a)] Corresponding author: sskraavi@phy.iith.ac.in*

Lead-free halide double perovskites have attracted significant attention as potential alternatives to toxic lead-based materials in optoelectronic applications. In this work, we investigate the effect of $Mn^{2+}$ doping on the scintillation behavior of $Cs_2AgInCl_6$ microcrystals. Samples with varying Mn concentrations were prepared via an acid precipitation approach utilizing halide-based precursors. Structural and compositional analyses, including XPS, confirmed successful Mn incorporation. Radioluminescence measurements revealed that Mn doping enhances the emission intensity, with the 10% Mn-doped sample showing optimal performance. The improved response is attributed to defect-assisted luminescence associated with aliovalent Mn doping. These findings demonstrate the promise of Mn-doped $Cs_2AgInCl_6$ as a lead-free scintillator material for X-ray detection and imaging.

**h0018**

**Modulated Electrical Transport in ZnO-ZnS Composite Nanorods**

Barnali Patra and Durga Basak*

*School of Physical Science, Indian Association for the Cultivation of Science, 2A and 2B Raja S.C Mullick Road, Kolkata 700032, India*

**Email: sspdb@iacs.res.in*

Quasi-vertically 1D ZnO nanorods (ZnO NRs) offer direct pathways for carrier transport along the c-axis, reducing scattering and enhancing electron mobility. ZnO–ZnS composite nanorods exhibit a remarkable enhancement in electrical conductivity as a result of significant improvements in both carrier concentration and mobility. Specifically, the carrier concentration increases by approximately 6.5 times, while the hall mobility rises by nearly 100 times compared to pristine ZnO NRs. This improved conductivity and mobility arises from increased donor defects and effective surface passivation via sulfur treatment. Photoluminescence (PL) studies further support this, showing a spectral shift from yellow-orange emission to green emission, which indicates formation of oxygen vacancies ($V_O$) type defects in ZnO-ZnS composites. Temperature-dependent resistivity measurements in ZnO–ZnS composites reveal two distinct conduction mechanisms. At higher temperature, transport is governed by thermally activated barrier conduction (TABC) and below 20 K conduction mechanisms shifts to nearest neighbor hopping (NNH) between localized donor states.

**h0020**

**Crystal Structure and Ionic Conduction of $K_2Ni_2Mo_3O_{12}$: A combined Neutron Diffraction and Impedance Spectroscopy Study**

K. B. Patel,[1,2] A. K. Bera[1,2 *] and S. M. Yusuf[1,2 *]

[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India;*

[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*

** akbera@barc.gov.in, smyusuf@barc.gov.in*

In the quest for economically and ecologically favorable solid-state electrolytes, we present here the detailed investigation of $K_2Ni_2Mo_3O_{12}$ (KNMO), as a potential K+ ion conducting solid electrolyte. Neutron and x-ray diffraction results reveal that K+1 occupy two distinct crystallographic Wyckoff sites; K1 and K2, within the open channels formed by edge sharing $NiO_6$ octahedra and $MoO_4$ tetrahedra. The soft bond valence sum analysis revealed two distinct one-dimensional conduction channels along the a and b axes, respectively. Impedance spectroscopy study over a broad temperature range (323–873 K) show the thermally activated nature of ionic transport with activation energy of 1.17(9) eV. The results establish KNMO as a model system for rationally designing next-generation potassium-ion conductors for all-solid-state energy storage applications.

**h0021**

**High Spectral Selectivity and Excellent Deep-UV Photosensitivity in a-$Ga_2O_3$ Film on Diverse Substrates**

Shantanu Jana and Durga Basak*

*School of Physical Science, Indian Association for the Cultivation of Science, 2A & B Raja S. C. Mullick Road, Jadavpur, Kolkata 700032, India*

**Email: sspdb@iacs.res.in*

Amorphous gallium oxide (a-$Ga_2O_3$) is an ultrawide bandgap semiconductor with strong potential for deep ultraviolet (UV) photodetectors due to its high UV absorption and stable optoelectronic properties. In this study room temperature RF-sputtered a-$Ga_2O_3$ thin films was deposited on fused quartz, single-crystal quartz, and glass substrates. The XRD study confirms their amorphous structure, while XPS reveals the presence of sub-stoichiometric phases. The sharp absorption below 280 nm and pronounced photosensitivity up to $2.2 \times 10^3$ under 250 nm illumination, confirms the ultrawide bandgap and high spectral selectivity of the films. The highest achieved responsivity of 41.3 mA/W and fast decay times (< 3 s) indicate balanced response with efficient carrier generation and recombination dynamics. Moreover, the transient responses remain consistent over multiple cycles, indicating excellent operational stability. Achieving such performance at room temperature offers a cost-effective, substrate-flexible route, reinforcing the potential of a-$Ga_2O_3$ thin films for next-generation deep-UV photodetectors and enabling large-area, low-temperature integration of high performance photosensors.

**h0022**

**Impedance Analysis of Manganese Orthophosphate Compound $Mn_3(PO_4)_2$**

Priyanka sharma[1,2], K. S. Chikara[1,2], Amit Kumar[1,2] and S. M. Yusuf [2,a]

[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India;*

[2]*Homi Bhabha National Institute, Mumbai 400094, India*
[a]Corresponding author: smyusuf@barc.gov.in
The complex impedance spectra of manganese orthophosphate, $Mn_3(PO_4)_2$, were measured by impedance spectroscopy over the temperature range of 323–873 K and at frequencies up to 1MHz. The single semicircular nature of the Cole–Cole plots indicates that the electrical response originates primarily from the bulk of the material. Further analysis reveals that the electrical behavior is frequency-dependent and thermally activated. Both DC and AC conductivities increase with temperature, indicating the semiconducting nature of the compound. The oxygen ion conductivity of $Mn_3(PO_4)_2$ is approximately $10^{-8}$ $S \cdot cm^{-1}$ at 323 K, increasing to about $10^{-4}$ $S \cdot cm^{-1}$ at 873 K. The relaxation process is governed by the intrinsic properties of the material and exhibits non-Debye characteristics. These results highlight the potential of $Mn_3(PO_4)_2$ as a promising model candidate for high-temperature ionic conduction processes.

**h0023**

**CoRuTiSn: A Low-Moment Narrow Band Gap Semiconductor**

Ravinder Kumar and Sachin Gupta[a]
*Department of Physics, Bennett University, Greater Noida 201310, India*
*[a] Corresponding author email: sachin.gupta@bennett.edu.in*
We report structural, magnetic and transport properties of quaternary Heusler alloy CoRuTiSn. The material crystallizes in tetragonal crystal structure at room temperature. Magnetic measurements indicate soft ferromagnetic behavior, with a Curie temperature around ~200 K. The saturation magnetic moment at 4 K was found to be ~0.84 $\mu_B/f.u.$. Temperature-dependent electrical resistivity and conductivity measurements confirm the semiconducting nature of the material. Fitting of the conductivity data reveals that the CoRuTiSn possesses a narrow band gap. Hall measurements show the presence of both ordinary and anomalous Hall contributions. Low moment semiconducting nature makes CoRuTiSn a promising candidate for semiconductor spintronics.

**h0024**

**Self-Powered UV Photodetector Based on Bandgap-Engineered Bi-Doped $Cs_2AgInCl_6$ Double Perovskite**

Chinmay Barman[1], Chinthala Sandeep Kumar[1], Sireesha Lavadiya[1], R. Sai Prasad Goud[2,3], S.V.S. Nageswara Rao[2,3], and Sai Santosh Kumar Raavi[1]*
*[1] Ultrafast Photophysics and Photonics Laboratory, Department of Physics, Indian Institute of Technology Hyderabad, Kandi 502285, Telangana, India*
*[2] Centre for Advanced Studies in Electronics Science and Technology (CASEST), School of Physics, University of Hyderabad, Hyderabad 500046, Telangana, India*
*[3] Centre for Nanotechnology, University of Hyderabad, Hyderabad 500046, Telangana, India*
**Corresponding author's e-mail address: sskraavi@phy.iith.ac.in*
The development of self-powered UV photodetectors is hindered by the lack of materials that simultaneously offer full-spectrum UV absorption and low-voltage operation. In this work, we demonstrate a self-powered UV photodetector based on Bi-doped $Cs_2AgInCl_6$, a lead-free double perovskite. $Bi^{3+}$ doping extends the absorption edge from 340 nm to 410 nm and introduces a sharp peak near 368 nm, attributed to Bi-induced s–p electronic transitions, enabling broad and efficient UV detection (250 – 410 nm). Beyond spectral tuning, Bi doping significantly improves carrier transport properties, enhancing mobility, extending carrier lifetime, and passivating deep-level defects. These improvements result in substantial enhancements in photocurrent, responsivity (0.34 A/W), detectivity ($1.76\times10^{13}$ Jones), and reduced dark current. The fabricated device operates effectively without external bias, exhibiting an ultrahigh open-circuit voltage of 0.66 V under 40 μW/cm² illumination. Furthermore, long-term ambient testing over three months shows only minor performance degradation, confirming excellent environmental stability. These findings establish Bi-doped $Cs_2AgInCl_6$ as a promising, environmentally friendly material platform for next-generation self-powered UV photodetectors.

**h0025**

**Effect of Ag Ion Irradiation on the Electrical Transport Properties of $La_{0.67}Sr_{0.33}MnO_3$ thin films**

Ramcharan Meena[1]*
*1. Inter University Accelerator Center, Aruna Asaf Ali Marg, New Delhi-110067.*
**Email: ramcharanmeena1992@gmail.com*
We report the effect of Swift Heavy Ion (SHI) irradiation (100 MeV Ag) on the structural and electrical transport properties of $La_{0.67}Sr_{0.33}MnO_3$ thin films deposited on Si-substrate. The irradiation is performed at two different ion fluences of 1E11 and 1E12 ions/cm$^2$. The structural analysis using the X-ray diffraction method shows, the strain present in the film released at higher fluences shows the annealing effect. The resistivity measurements show the metal-insulator transition in all samples, with an overall decrease in resistivity in a magnetic field of 0.2 T, confirming the negative magneto-resistance behavior. Metal-Insulator (M-I) transition temperature increases towards higher temperatures at initial fluence and decreases for higher fluence. The experimental data at low temperature below $T_{min}$ are fitted using the Kondo-like expression and the metallic-like conductivity expression above the minimum temperature. The observed increase in resistivity is explained using ion beam-induced defects in the LSMO thin films. The negative magneto-resistance is explained by the suppression of magnetic domain boundary scattering of charge carriers by a magnetic field.

**h0026**

**Electronic Band Structure and Thermoelectric Behavior of LiScSn: A First-Principles Approach**

Dipti Gawande[1*], Shubha Dubey[1], Archana Srivastava[2], Gitanjali Pagare[3], N. K. Gaur[1]
[1] *Department of Physics, Barkatullah University, Bhopal 462 026, India*
[2] *Department of Physics, Shri Sathya Sai College for Women, Bhopal 462 024, India*
[3] *Department of Physics, Sarojini Naidu Govt. Girl P.G. Autonomous College, Bhopal 462016, India*
** Corresponding author: diptigawande5@gmail.com*

In the present study, we have systematically investigated the structural, electronic, and thermoelectric properties of LiScSn using the full-potential linearized augmented plane wave (FP-LAPW) method within the WIEN2k framework. Structural optimization was performed using the Perdew–Burke–Ernzerhof generalized gradient approximation (PBE-GGA), ensuring reliable equilibrium lattice parameters. To obtain a more precise description of the electronic structure, both PBE-GGA and the Tran–Blaha modified Becke–Johnson (TB-mBJ) potential were employed. Our results indicate that LiScSn is an indirect semiconductor, exhibiting band gaps of approximately 0.6 eV within PBE-GGA and 0.9 eV within the TB-mBJ scheme, demonstrating the significant improvement in gap prediction with the latter. Furthermore, the thermoelectric performance of LiScSn was assessed by evaluating the dimensionless figure of merit (ZT), which was found to be close to unity. This value highlights the promising efficiency of LiScSn for thermoelectric applications. The combination of a moderate band gap, favorable electronic transport properties, and a ZT near 1 suggests that LiScSn can serve as a potential candidate for both thermoelectric energy conversion applications.

**h0028**

**Thermopower in a Correlated Disordered 1D Chain**

Shweta Kumari[1*], Santanu K. Maiti[2], Surender Pratap[1]
[1]*Deparment of Physics and Astronomical Sciences, Central University of Himachal Pradesh, Dharamshala-176 215, India*
[2]*Physics and Applied Mathematics Unit, Indian Statistical Institute, 203 Barrack, Kolkata-700 108, India*
**shwetashweta444@gmail.com*

We investigate thermoelectric transport properties of a one-dimensional (1D) tight-binding chain subject to correlated quasiperiodic modulations in on-site energies and nearest-neighbor hopping integral. This is achieved by combining the Aubry–Andre–Harper (AAH) model, which modulates site energies and hopping integrals, with the Su–Schrieffer–Heeger (SSH) model, which features alternating hopping parameters ($t_1 \neq t_2$). Employing the Landauer–Büttiker formalism, we compute both the electronic and phononic transmission functions and evaluate the Seebeck coefficient (S) as a function of chemical potential ($E_F$). Our analysis focuses on the off-diagonal generalized AAH model and its interplay with SSH-type disorder. We observe a significant enhancement in the S when transitioning from the pure AAH model to the correlated AAH + SSH disordered system, highlighting the role of structural modulation and electronic localization in optimizing thermoelectric performance at the nanoscale.

**h0029**

**Studies on Growth morphology of Germanium Single crystal**

P Dixit[1], S.G. Singh[1, 2, a], A.K. Singh[1], G.D. Patra[1, 2,] M. Ghosh[1], S. Pitale[1], S. Sen[1, 2, b]
[1]*Technical Physics Division, Bhabha Atomic Research Centre, Mumbai 400085*
[2]*Homi Bhabha National Institute, Mumbai 400094*
*Corresponding author: sgovind@barc.gov.in, shash@barc.gov.in*

High Purity Germanium (HPGe) detectors are widely used for gamma-ray spectroscopy due to their superior energy resolution. To make HPGE detectors high-quality single crystals of germanium is required. We have grown Ge single crystals using the Czochralski (CZ) method in hydrogen ambient with a flow rate of 1 L/min. In this work, we optimized the axial thermal gradient by changing the growth station like adjusting the dimensions of the crucible and susceptor, and validated the thermal profile using COMSOL simulations for two configurations. The resulting crystal showed excellent shape and structural quality. Crystallinity was evaluated using HRXRD rocking curves, dislocation density was measured via etch pit density, and electrical transport properties were characterized using van der Pauw Hall measurements.

**h0030**

**Structural and Transport Behavior of Kagome metal $YMn_6Sn_6$**

*Ramendra Gupta, H. Pradhan, Anuj Kumar, A. G. A. Rahman, A. Awasiya, R. K. Patel and A. K. Pramanik.*
*School of Physical Sciences, Jawaharlal Nehru University, New Delhi, 110067*
**Email:guptaramendra042@gmail.com*

We have studied the structural, electronic transport properties and temperature dependent Current (I) -Voltage (V) characteristic of Kagome metal $YMn_6Sn_6$. The solid-state reaction method was used to synthesized the sample. Structural characterization was carried out using X-ray powder diffraction (XRD) and Rietveld analysis which reveals Hexagonal crystal structure with P6/mmm space group. Electrical resistivity measurement is done using four-probe method, which shows that $YMn_6Sn_6$ exhibit metallic behavior throughout the temperature range. The I-V characteristic becomes non-linear below 200K due to charge trapping, tunneling barriers, Schottky-type contacts, or electron localization. This electronic charge transport behavior found to follow power law dependence in low temperature

**h0032**

**Suppression of Surface Oxidation in Copper Nitride Films Through Chromium Nitride Capping for Transport Properties.**

Madhu S[1], Warrier Sivaprasad U. L[1]., Ashok Rao[2], Kodihalli K. Nagaraja[1,*]

*[1]Alternative Energy Materials Lab, Department of Physics, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal,576 104, India.*

*[2]Functional Materials Lab, Department of Physics, Manipal Institute of Technology, Manipal, Manipal Academy of Higher Education, Manipal,576104, India.*

**Email:nagaraja.kk@manipal.edu: nrajkk@gmail.com*

Sputtered Copper Nitride ($Cu_3N$) thin films deposited by are highly susceptible to atmospheric oxidation, leading to changes in electrical properties over time. While X-ray diffraction analysis showed only $Cu_3N$ crystalline peaks without detectable copper oxide phases, Raman spectroscopy revealed the presence of copper oxide phases on the film surface, indicating surface oxidation. In an effort to mitigate this oxidation issue, we explored the deposition of a thin Chromium Nitride (CrN) protective layer (~20 nm) as a capping layer on the $Cu_3N$ films. Raman spectroscopy of the CrN-capped (CP60s) showed complete suppression of copper oxide peaks. XPS depth profiling confirmed the effectiveness of the CrN capping layer in preventing oxygen diffusion to the $Cu_3N$ surface. Most importantly, electrical resistivity measurements demonstrated excellent stability over months of atmospheric exposure for the CrN-capped $Cu_3N$ films and the power factor of 38.4 $\mu W \cdot m^{-1} \cdot K^{-2}$ was obtained. The results indicate that a thin CrN capping layer provides effective protection against oxidation. This approach offers a practical solution for improving the surface stability of $Cu_3N$ for electronic devices in ambient conditions and for thermoelectric applications.

**h0033**

**Thermoelectric Properties Of Twisted Graphene and Boron Nitride Heterostructure: A First Principles Study**

Prasann S Kshatriya and Yogesh A Sonvane*

*Advanced Materials Lab, Department of Physics, Sardar Vallabhbhai National Institute of Technology, Surat, 395007, India*

**Email:yas@phy.svnit.ac.in*

In this work we present a first-principles investigation of thermoelectric properties of 32.2° twisted Graphene/ Boron Nitride heterostructure. We have employed Density Functional Theory (DFT) and Boltzmann Transport Theory within the Constant Relaxation Time Approximation. We have calculated the electronic band structure, Seebeck Coefficient, electrical conductivity as well as lattice thermal conductivity and have estimated the thermoelectric figure of merit ZT. We observe suppressed lattice thermal conductivity for this system which is less than 4 W/mK. The maximum obtained lattice thermal conductivity is 3.58 W/mK at 400 K. Although Lattice Thermal conductivity is quite low we find that electron's contribution to thermal conductivity tends to dominate at temperatures larger than 650 K eventually reducing the Thermoelectric figure of merit ZT to 0.2. We also obtain a small band-gap of 0.05 meV which is due to the moire effects introduced in the system. This makes this a system a promising candidate to explore strain engineering, defect scattering, bandgap tuning etc in order to improve its thermoelectric performance

**h0035**

**The Structural, Morphological and Optical Properties of β- $Ga_2O_3$ Nanorods grown by Facile Hydrothermal method**

**Nidhi Khare, Alwin Scaria Shelly and R. Thangavel**

*Semiconductor Research and Device Lab, Department of Physics, Indian Institute of Technology (ISM) Dhanbad 826004, Jharkhand, India.*

**Email:rthangavel@iitism.ac.in*

β-$Ga_2O_3$ is the most unique ultra-wide bandgap material having bandgap `4.8eV, higher critical electric field `8MV and higher Baliga Figure of Merit~ 3000 which make it most suitable candidate for power electronics and optoelectronic applications. In this work β- $Ga_2O_3$ nanorods with monoclinic phase and space group C2/m, have been grown by facile hydrothermal method. The grown β- $Ga_2O_3$ nanorods are having dimension with Average length 975nm and average width 325nm respectively. The β- $Ga_2O_3$ nanorods shows a ultra-wide bandgap of around 4.7eV and reflect the 81% of Visible-NIR Radiation and absorb UV radiation around 265 nm.

**h0036**

**Exploring Photothermal Effects on Current Modulation in F8BT Thin Films**

*Sirsendu Ghosh, Pramod Kumar[a]*

*Department of Physics, Indian Institute of Technology Bombay, Mumbai, 400076, India*

*[a)]Corresponding author: pramod_k@iitb.ac.in*

In this letter, we have demonstrated photothermal modulated current phenomena in Poly9,9-dioctylfluorene-alt-benzothiadiazole (F8BT) polymer at a bias of 10 μV when light as an external stimulation which consists of ultraviolet (UV) to infrared (IR) broad-spectrum incident on it. F8BT shows some atypical behavior with ephemeral existence of light. The sudden increase of current with immediate decay by applying the light and the sharp spike of the current in the opposite direction in the absence of light below the dark current indicates the analogy with the pyro-phototronic effect. The F8BT absorbs UV light, while the IR component of the spectrum contributes to heating effects, creating a temperature gradient between the ITO and PEDOT: PSS electrodes. This interplay between photoinduced charge generation and thermally driven transport leads to the observed transient characteristics. Photogenerated charge carriers, presence of trap states in the F8BT, and temperature difference between the electrodes due to the IR are responsible for this type of behavior which is the new direction in organic semiconductor (OSC) physics, will be explored more in near future.

**h0037**

**Effect of MWCNT Based Source and Drain Contacts in Organic FETs**

Priyanshu Kunwar[1,*], Ramesh Singh Bisht[1], Sirsendu Ghosh[1], Mayank Pal[1], Kiran M. Subhedar[2], Pramod Kumar[1]

[1]*Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India*

[2]*CSIR-National Physical Laboratory (NPL), New Delhi, 110012, India*

[*]*Corresponding author: priyanshu_kunwar@iitb.ac.in*

This work explores the effect of using multi-walled carbon nanotube (MWCNT) yarns as source and drain electrodes in organic field-effect transistors (OFETs), replacing traditional Au/Ag or other metal contacts. The device was fabricated using spin-coated PBTTT-C14 thin film and chemical vapor deposition (CVD) grown MWCNT yarns. Electrical measurements revealed device transfer characteristics and mobility behavior. Simulations were conducted using a hopping percolation model assuming an exponential density of states. While the theoretical model showed a linear mobility dependence on carrier density (on a log-log scale), experimental results displayed a nonlinear behavior. This mismatch can be attributed to a dynamic barrier between MWCNT electrodes and the organic semiconductor due to the gate field. The findings highlight MWCNTs' potential in flexible electronics and emphasize the need to account for contact effects in modelling.

# i) Magnetism and superconductivity

**i0001**

**Role of Crystal Structure on the Multiscale Magnetic Properties of Correlated Double Perovskites $La_2Mn_{2-x}Ni_xO_6$**

A. K. Bera[1,2,a] and K. S. Chikara[1,2]

[1] *Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, India.*

[2] *Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India.*

**Email: akbera@barc.gov.in (Email of corresponding author)*

The magnetic correlations in $La_2Mn_{2-x}Ni_xO_6$ ($x$ = 0.5–1.5) were systematically studied across multiple length scales using DC magnetization, neutron depolarization, and neutron powder diffraction. With increasing Ni content, the system evolves from long-range ferromagnetic (FM) order to cluster ferromagnetism and spin-glass (SG) behavior, driven by structural transitions from orthorhombic ($x$ = 0.5) to mixed orthorhombic–monoclinic ($x$ = 0.75–1.0) and finally monoclinic–trigonal ($x$ = 1.25–1.5) phases. The FM ordering temperature increases from 170 K ($x$ = 0.5) to 280 K ($x$ = 1.0), but magnetization and ordered moment decline, with long-range order vanishing beyond $x$ = 1.0. All compositions show a low-temperature reentrant SG-like phase below ~50 K. Neutron diffraction confirms that long-range FM order is confined to the orthorhombic phase. These results reveal how structural evolution governs the tunable magnetism in $La_2Mn_{2-x}Ni_xO_6$, informing the design of spintronic materials.

**i0002**

**Study of Dielectric & Ferroelectric Behavior in Mn Modified $BaTiO_3$**

Rony Kohli[1, a)], Shivani Kulasari, Ayush Rana, Piyush Singh, Om Prakash, and Sanjay Kumar Upadhyay

*HNB Garhwal University Srinagar-Garhwal-246174, Uttarakhand, INDIA*

**Email:ronykohli21@gmail.com*

In the present work, Mn-doped barium titanate, $BaTi_{1-x}Mn_xO_3$ (x=0.02, 0.05), was studied by means of x-ray diffraction, ferroelectric, and dielectric measurements. Phase-coexistence (tetragonal and hexagonal) has been observed for both compositions. For x= 0.02, a pinched type of ferroelectric hysteresis loop has been observed due to the presence of defect dipole. The origin of the defect dipole can be understood in terms of the generation of oxygen vacancies, created by the charge imbalance of $Ti^{4+}$ and $Mn^{3+}$. The transition temperature for x= 0.02 sample comes out to be 395 K. For x= 0.05 sample, typical paraelectric behavior has been observed in PE loop at room temperature. However, the transition temperature comes out to be 391 K in temperature-dependent dielectric data, essentially associated with a small fraction of tetragonal phase.

**i0003**

**Experimental Realization of Magnon Modes in the Trimerized Collinear-II Antiferromagnet $Li_2Ni_3P_4O_{14}$**

K. S. Chikara, A. K. Bera, A. Kumar, and S. M. Yusuf

*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India;*

*Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*

**Email: akbera@barc.gov.in, amitkr@barc.gov.in*

We report the magnetic ground state and spin excitations of the 2D spin-1 trimerized Heisenberg antiferromagnet $Li_2Ni_3P_4O_{14}$. Below the Néel temperature (TN = 14.5 K), it exhibits a canted antiferromagnetic order with propagation vector k = (0 0 0) and magnetic space group P21/c.1(#14.75). The ground state comprises ferromagnetic spin-trimers of $Ni^{2+}$ ions, coupled antiferromagnetic (AFM) along the c-axis and ferromagnetic (FM) along the a-axis. Inelastic neutron scattering spectra reveal gapped and dispersive magnon modes below TN. Spin-wave simulations capture the spectrum using a Hamiltonian with FM intra-trimer ($J_1$) and inter-trimer couplings ($J_2$ FM, $J_3$ AFM) with exchange ratios of $J_2/J_1 = 0.79$, $J_3/J_1 = -0.91$. A weak interlayer FM $J_4/J_1 \approx 0.12$ exchange interaction along the a-axis is found. This confirms a 2D trimerized Collinear-II lattice in the bc-plane. A moderate single-ion anisotropy ($D/J_1 = 0.48$) explains the observed spin gap and metamagnetic behavior. The results provide direct experimental evidence of theoretically predicted magnon excitations in the class of 2D trimer spin system in the strong exchange coupling range. In summary, $Li_2Ni_3P_4O_{14}$ thus emerges as a rare realization of model system for 2D trimerized collinear-II lattice.

**i0004**

**Insights about the structural and physicochemical properties of $(CuNiTiZnFe)_3O_4$**

Sakshi Kaundal [a)] and K. Mukherjee

*School of Physical Sciences, Indian Institute of Technology Mandi, Kamand,175075 (HP) India*

*[a)] Corresponding author: sakshikaundal501@gmail.com*

Spinel oxides present an intriguing avenue for investigating magnetic interactions and electron correlations, owing to their adaptable structure and the existence of transition metal ions exhibiting various oxidation states. Recently, there has been an increasing focus on high entropy spinel oxides (HESOs), given that their chemical complexity can result in a diverse array of adjustable and unconventional magnetic properties. This study presents the successful synthesis of a single-phase HESO of the composition $(CuNiTiZnFe)_3O_4$. This system crystallizes into a cubic structure with a lattice constant of 8.4095(3) Å, and there is an angular distortion of $\pm 3.589°$ at octahedral site. The X-ray photoelectron spectroscopy study revealed the presence of magnetic $Cu^{2+}$, $Ni^{2+}$, $Ni^{3+}$, $Ti^{3+}$, Fe2+, and Fe3+ along with non-magnetic $Zn^{2+}$, $Ti^{4+}$ oxidation states of constituent cations of this high entropy oxide. Also, there is a presence of some oxygen vacancies, which are essential to stabilize the configuration.

**i0005**

**Effect of $Ni^{2+}$ Incorporation on Phase Formation and Multifunctional Properties of $SrFe_{12-x}Ni_xO_{19}$ Hexaferrites**

Sher Singh Meena[1,*], N. Maramu[2] and Sadhana Katlakunta[3] , Ch. Srinivas[4]
[1]*Solid State Physics Division, Bhabha Atomic Research Center, Mumbai 400 085, India*
[2]*Department of Physics, Kakatiya Institute of Technology and Science, Warangal-506015, Telangana, India*
[3]*Department of Physics, University College of Science, Saifabad, Osmania University, Hyderabad-500004, Telangana, India*
[4]*JNTU-K Research Centre-Nanomaterials and Nanomagnetism Research Laboratory, Department of Physics, Sasi Institute of Technology & Engineering, Tadepalligudem 534101, Andhra Pradesh, India*
[*]*Email: ssingh@barc.gov.in*
$SrFe_{12-x}Ni_xO_{19}$ (where $x$ = 0.0–1.0 in steps of 0.2) samples were synthesized via the co-precipitation method and sintered at 1100 °C for 4 hours. The structural, morphological, magnetic, and hyperfine interaction properties were systematically investigated at room temperature. With increasing $Ni^{2+}$ content, the lattice parameters 'a' and 'c' exhibited a gradual increase. SEM analysis revealed that the grains possess a hexagonal plate-like morphology, and the average grain size decreased with $Ni^{2+}$ substitution. The average grain size (<*D*>) ranged from 1.713 μm ($x$ = 0) to 0.549 μm ($x$ = 1.0). Saturation magnetization ($M_S$) decreased from 68 emu/g ($x$ = 0.0) to 50 emu/g ($x$ = 0.6), followed by an increase to 64 emu/g at $x$ = 0.8. Both $M_S$ and <*D*> exhibited similar trends with Ni substitution, suggesting a correlation between microstructural and magnetic behavior. Coercivity ($H_C$) varied anisotropically with increasing Ni content. The squareness ratio ($M_r/M_S$) remained above 0.56 for all compositions, indicating the presence of a single-domain structure. Mössbauer spectroscopy confirmed that all Fe ions exist in the high-spin $Fe^{3+}$ state, with no evidence of $Fe^{2+}$ across the series. The dielectric constant ($\varepsilon'$) and dielectric loss (tan $\delta$) were found to increase with $Ni^{2+}$ doping at room temperature. Based on the observed structural, magnetic, and dielectric properties, it can be concluded that $SrFe_{12-x}Ni_xO_{19}$ M-type hexaferrites are promising candidates for microwave device applications.

**i0006**

**Critical Behavior and Chiral Magnetic Phases in Single Crystalline Mn Intercalated $TaS_2$**

Tuhin Debnath[1], Mintu Mondal[1*]
[1]*School of Physical Sciences, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700032, India*
**Email: sspmm4@iacs.res.in (Email of corresponding author)*
Chiral magnetic solitons with unique topological spin textures have potential in spintronics for developing highly stable, efficient, and low-power devices. The chiral magnetic phases in Mn intercalated $TaS_2$ compound, a potential candidate for hosting chiral magnetic soliton phase, have been investigated via critical scaling analysis of isothermal magnetization across the ferromagnetic to paramagnetic transition. This compound shows a ferromagnetic (FM) order below $T_C \approx 30$ K and exhibits magnetic anisotropy with a large ab-plane moment and a small moment along the c-axis. The critical scaling analysis of isothermal magnetization yields the critical exponents $\beta = 0.377 \pm 0.002$, $\gamma = 1.345 \pm 0.003$, $\delta = 4.682 \pm 0.003$. The exponent $\beta$ is close to the 3D Heisenberg model but $\gamma$ lies between the 3D Heisenberg and 3D XY models, suggesting the presence of complex magnetic interactions. Two points of inflection have been identified from the renormalized Arrott plot using the obtained critical exponents. Based on this study, we have reconstructed the magnetic phase diagram demonstrating the emergence of a chiral helimagnetic phase (CHM), a chiral magnetic soliton lattice phase (CSL), and a forced ferromagnetic phase in single crystalline Mn intercalated $TaS_2$.

**i0007**

**Understanding The Role Of Fe Doping On Magnetism In $Cr_2CoSb$ Heusler Alloy: Insights From First Principles Calculations**

Aisha Iftikhar[1,2], K.S Chikara[1,2], A. Kumar[1,2*]
[1] *Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, INDIA*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai-400094, INDIA.*
** amitkr@barc.gov.in(Email of corresponding author)*
We present a first-principles investigation of the structural, electronic, and magnetic properties of Fe-substituted Heusler alloys $Cr_{2-x}Fe_xCoSb$ ($x$ = 0 – 1) using DFT-based calculations. The parent compound exhibits a high spin polarization (~94%) and a magnetic moment of ~2.0 $\mu_B$/f.u., with a stable FCC structure (space group $F\bar{4}3m$). Fe substitution leads to a systematic decrease in lattice parameter and an increase in magnetic moment, reaching ~4.0 $\mu_B$/f.u. for $x$ = 1. Density of states analysis reveals that Fe doping shifts the Fermi level toward the valence band of the minority spin channel, reducing spin polarization. This behavior is attributed to electron doping by Fe atoms. The results highlight the trade-off between magnetic moment enhancement and spin polarization reduction. Our findings provide insight into tuning Heusler alloys for spintronic applications. These calculations may guide future experimental efforts for the design of materials for spintronic applications.

**i0008**

**Disorder-Tuned Quantum Phase Transition in Nanoporous NbN Thin Films**

Amar Verma[1, a)] and Sangita Bose[1, b)]
[1]*School of Physical Sciences, UM-DAE Centre for Excellence in Basic Sciences, University of Mumbai, Kalina campus, Santacruz (E), Mumbai 400098, INDIA.*
[a)] *Corresponding author: amar.verma@cbs.ac.in*
Quantum phase transitions (QPT) in low-dimensional systems offer a powerful framework for understanding ground-state properties governed by non-thermal parameters such as disorder, magnetic field, or carrier density. In two-dimensional (2D) superconductors, increasing disorder can drive a superconductor–insulator transition (SIT), where long-range phase coherence is

destroyed and the system evolves toward an insulating state as the sheet resistance approaches the quantum resistance $R_Q = h/4e^2$ (6.45 kΩ). In this work, we investigate disorder-tuned SIT in NbN films deposited on nano-porous anodic aluminum oxide (AAO) substrate featuring 40 nm diameter pores with 100 nm lattice spacing. By utilizing both the top (granular) and bottom (more uniform) surfaces of the AAO substrate, we introduce distinct disorder landscapes within the same material system. A clear SIT is observed with decreasing film thickness, underscoring the critical role of disorder and quantum fluctuations. Remarkably, vortex matching effect (VME) signatures persist even in the insulating regime, indicating the presence of localized Cooper pairs and supporting a bosonic mechanism for the SIT.

**i0009**

**Disorder-Tuned Superconducting Behavior in Nanocrystalline $Nb_xSn_{1-x}$ Thin Films**

Mahesh Poojary[1, a)] and Sangita Bose[1, b)]
[1]*School of Physical Sciences, UM-DAE Centre for Excellence in Basic Sciences, Mumbai 400098, India.*
*mahesh.poojary@cbs.ac.in*

In this study, we investigate the evolution of the $Nb_xSn_{1-x}$ thin films by systematically tuning disorder through compositional variation and film thickness. Two series of films were grown using DC magnetron sputtering: one stoichiometric $Nb_3Sn$ (75:25) and another off-Stoichiometry $Nb_{2.5}Sn$ (72:28). Growth conditions were optimized which gave a $T_c$ of 17.8 K for the thickest film. The structural disorder was quantified using XRD. $Nb_3Sn$ A15 phase was seen to form in films down to the lowest thickness for both series. However, subtle differences emerge in the off-stoichiometric series, which shows stronger sensitivity to dimensional tuning due to its higher intrinsic disorder. Both series display a suppression of $T_c$ with decreasing thickness, but the effect is significantly more pronounced in the disordered $Nb_{2.5}Sn$ films. These findings offer valuable insight into how disorder influences superconductivity at the nanoscale and provide a foundation for studying quantum phase transitions in disordered superconducting systems.

**i0010**

**Terahertz Spectroscopy of LZNFO nanoparticles**

Anol Mondal;[1a)], Anushka Kshirsagar[1], Sudeep Tiwari[1b)] and S.S.Prabhu[1]
[1]*Tata Institute of Fundamental Research, Mumbai,400005, India*
*Corresponding author email : [a)] anol.mondal2002@gmail.com [b)] sudeep.tiwari@tifr.res.in*

LZNFO nanoparticles were synthesized using sol-gel method with the particle size about 28 nm. The nanoparticles, as confirmed via PXRD, exhibit fcc-spinel structure with cationic distribution $[Zn^{2+}_{0.25}Fe^{3+}_{0.75}]_A[Li^{+}_{0.5}Fe^{3+}_{1.25}Ni^{2+}_{0.10}\ Ni^{3+}_{0.15}]_B$. The study focusses on the optical response of these nanoparticles in the THz region. The optical properties of the nanoparticles were investigated using the Terahertz Time Domain Spectroscopy (THz-TDS), which reveals a refractive index of about 2.6. The time domain outcome of conductivity and dielectric constant shows the existence of multi-mode excitations, which are properly fitted using Drude-Lorentz and Lorentz three oscillator model respectively. A low value of loss tangent hints at the possibility of using this material for THz antenna miniaturization.

**i0011**

**Investigation of Vortex Response at low AC excitation in $Fe_xSe_{1-x}$ Thin Films through Electrodynamic Measurements**

Ekta Kadam[1] and Sangita Bose[1*]
[1]*School of Physical Sciences, UM-DAE Centre for Excellence in Basic Sciences, University of Mumbai, Kalina campus, Santacruz (E), Mumbai 400098, INDIA.*
**Email: ekta.kadam@cbs.ac.in*

We studied the vortex response in $Fe_xSe_{1-x}$ thin films using low frequency electrodynamic measurements with a two-coil mutual inductance technique at low AC excitation currents. The complex penetration depth was analyzed using the Gittleman-Rosenblum (GR) model to understand vortex dynamics and pinning mechanism. Parameters such as the Labusch parameter and vortex viscosity were obtained, revealing field-dependent behavior indicative of strong random pinning. The extracted vortex viscosity values were higher than those predicted by the Bardeen-Stephen model, suggesting that further theoretical models need to be studied to understand vortex response in the studied $Fe_xSe_{1-x}$ thin films.

**i0012**

**Impact of Transition Metal Substitution (Cu, Zn) at The M Site in $La_2(Ni/Co)_{1-x}M_xMnO_6$**

K. Jeevanandham, K. Vinod [a)] A. T. Sathyanarayana, and Awadhesh Mani
*Condensed Matter Physics Division, Materials Science Group, Indira Gandhi Centre for Atomic Research, A CI of Homi Bhabha National Institute, Kalpakkam, Tamil Nadu – 603102.*
*[a)] Corresponding author: vinod@igcar.gov.in*

Electronic transport properties of the $La_2(Ni/Co)_{1-x}M_xMnO_6$ (M = Cu, Zn) series were investigated using a dipstick setup in conjunction with a liquid nitrogen system over the 77–300 K range. Semiconducting behavior was observed across all compositions. Substitution of Cu and Zn at the Ni/Co site significantly affected the resistivity, suggesting that cationic substitution influences charge transport in these double perovskites.

**i0013**

**Probing Pair-Density Waves in Cuprates: Theory of Josephson Scanning Microscopy with an s-wave Tip**

Monikana Gope*, Shashwat Chaturvedi, and Peayush Choubey
*Department of Physics, Indian Institute of Technology Roorkee, Roorkee 247667, Uttarakhand, India*
**monikana1999@gmail.com*

Identifying a pair-density wave (PDW) in strongly correlated superconductors remains a significant challenge, both experimentally and theoretically, particularly when its wavevector coincides with that of other competing orders, such as charge-density waves (CDW), spin-density waves (SDW), etc. Scanned Josephson Tunneling Microscopy (SJTM) – a variant of scanning tunneling microscopy (STM) which measures Josephson and quasiparticle tunneling current between a superconducting tip and a superconducting sample- is a direct local probe of superconducting gap order parameter $\Delta(\mathbf{r})$, and hence, most suitable for detecting pair density waves (PDW) characterized by periodically modulating $\Delta(\mathbf{r})$. In this work, we resolve this issue by developing a first-principle Wannier function-based approach to calculate critical Josephson tunnelling current and comparing these with STM responses for Bi2Sr2CaCu2O8+ δ. In addition to this, we will compute the resulting quasiparticle interference (QPI) patterns alongside the SJTM response by introducing a non-magnetic impurity (e.g., Zn). This combined approach provides a robust framework for unambiguously identifying the presence of PDW order.

**i0014**

**Single Crystal Growth, Magnetic and Electric Properties of $Eu_5Sn_2As_6$**

Deepak. Kumar[1], R. Kalaivanan[2], R. Sankar[2] and I. Panneer Muthuselvam,[1,3, *)]
[1]*Department of Physics, Banaras Hindu University, Uttar Pradesh-221005, India*
[2]*Institute of Physics, Academia Sinica, Taipei 10617, Taiwan*
[3]*Department of Physics & Astrophysics, University of Delhi, Delhi-110007, India*
**Email: ipmphysics@bhu.ac.in*

High-quality single crystals of $Eu_5Sn_2As_6$ were synthesized via the self-flux method, yielding a well-ordered orthorhombic crystal structure. Temperature-dependent magnetic susceptibility $\chi(T)$ measurements identify it as a canted antiferromagnet below 10.04 K. Electrical resistivity $\rho(T)$ measurement reveals a metal-to-insulator transition observed just below room temperature (RT) with a narrow activation energy of 66.2 meV.

**i0015**

**Magnetic Properties of Non-Centrosymmetric $EuPtSi_3$ Single Crystals.**

Ruta Kulkarni* and A Thamizhavel
*Department of Condensed Matter Physics & Materials Science,*
*Tata Institute of Fundamental Research, Homi Bhabha Road, Mumbai-400005, India*
**Email: *ruta@tifr.res.in*

We report on the single crystal growth of $EuPtSi_3$, a non-centrosymmetric compound, which crystallizes in the $BaNiSn_3$-type crystal structure. The tetragonal crystal structure possesses only one Eu-site in the unit cell. The crystal growth of $EuPtSi_3$ is accomplished by the flux growth method using molten Sn as flux. From the detailed magnetic studies, it was found that $EuPtSi_3$ is an antiferromagnet with two successive magnetic transitions at $T_{N1}$ = 17 K and $T_{N2}$ = 16 K. These magnetic transitions were further confirmed by the heat capacity measurements as well. In the magnetically ordered state, the isothermal magnetization data for H // [001] exhibited a metamagnetic transition at around 1 T, with further increase in the magnetic field, magnetization achieved a saturation value of 6.43 $\mu_B$/Eu and the saturation along the [100] direction was achieved in a field of about 5.9 T.

**i0016**

**Field-induced ultrasharp staircase-like magnetization jumps 40% Cu doped $UMn_2Ge_2$ intermetallic compound**

Buddhadev Kanrar[1, *], Srikanta Goswami[2, 3], P.D. Babu[2]
[1]*Fuel Chemistry Division, Bhabha Atomic Research Centre, Mumbai, 400085*
[2]*UGC-DAE Consortium for Scientific Research, Mumbai Centre, BARC, Mumbai, India 400085*
[3]*FZU - Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, 182 21 Prague 8, Czechia*
[*] *Corresponding author: buddha@barc.gov.in*

The intermetallic compound $U(Mn_{0.6}Cu_{0.4})_2Ge_2$ synthesised by arc melting and characterized by X-Ray Diffraction. The main controlling parameters of magnetism in this system, the uranium-uranium distance ($d_{U-U}$) and uranium and transition metal distance ($d_{U-T}$), are altered by the substitution of Cu for Mn, which give raise antiferromagnetic (AFM) order from ferromagnetic order of parent compound. A 40% doping of Cu in place of Mn leads a robust antiferromagnetism in this compound and exhibits sharp magnetization jumps as field is swept at 3K. The compound exhibits AFM order below 200K and ferromagnetic order between 200K to $T_C$ ~ 325K. It also exhibits 37% Griffiths phase well above $T_C$.

**i0017**

**Synthesis, Magnetic and Dielectric properties of $SrMn_{0.8}Te_{1.2}O_6$ with mixed valency of $Mn^{3+}/Mn^{4+}$**

[1]Arpita Rana, [2]Ankita Mohanty, [2]A. K. Singh and [1,3,*]I. Panneer Muthuselvam
[1]*Department of Physics(MMV), Banaras Hindu University, Varanasi, Uttar Pradesh- 221005, India*
[2]*Department of Physics & Astronomy, National Institute of Technology Rourkela, Odisha- 769008, India.*
[3]*Department of Physics & Astrophysics, University of Delhi, Delhi-110007, India.*

* *ipmphysics@gmail.com*
We report a comprehensive study of the structural, magnetic, and dielectric properties of the $SrMn_{0.8}Te_{1.2}O_6$. Rietveld refinement result confirms the formation of a single-phase with tetragonal structure of lattice parameters, $a = b = 5.0932$ Å and $c = 5.3792$ Å. Magnetic susceptibility measurements disclose a Curie-Weiss-like paramagnetic behavior over a wide temperature range and reveal subtle features pointing to weak magnetic interactions at low temperatures. Isothermal magnetization curves at 2 K show nearly linear dependence without significant hysteresis, indicating the predominance of antiferromagnetically correlated paramagnetic features. Dielectric measurements exhibit a broad and monotonic enhancement in permittivity with rising temperature, and a pronounced frequency-dependence in both permittivity and dielectric loss, with moderate suppression under magnetic field. These results suggest an interplay between the lattice, spin, and charge degrees of freedom in $SrMn_{0.8}Te_{1.2}O_6$.

**i0018**

**Temperature – Driven Evolution from Short-Range Ferromagnetic Clusters to Glassy State in $TbCoC_2$**

Manisha Choudhary* and K. Mukherjee
*School of Physical Sciences, Indian Institute of Technology Mandi, Mandi 175075, Himachal Pradesh, India*
**manishachoudhary092002@gmail.com*

We investigate the magnetic properties of a rare-earth based dicarbide $TbCoC_2$ that crystallizes in a non – centrosymmetric orthorhombic structure. DC susceptibility confirms the presence of high temperature transition followed by a ferromagnetic (FM) transition at 28 K. Below this FM transition, significant drop in moment and a bifurcation between zero field cooled and field cooled curve suggests towards the presence of disordered magnetic state. A combined DC and AC susceptibility study indicate that the high temperature transition can be attributed to the dynamical short-range FM cluster state in paramagnetic matrix. The dynamic magnetization studies provide the evidence of cluster glass state below FM transition.

**i0019**

**Supper Paramagnetic Behavior of Ni-Mn-Ga Melt Spun Ribbon**

A. Satish Kumar[1, a], M. Ramudu[2] and V. Seshubai[3]
[1]*Department of Physics, Rajiv Gandhi University of Knowledge Technologies- Nuzvid-521201, India*
[2]*School of Sciences (Physics), National Institute of Technology, Andhra Pradesh-534101, India*
[3]*School of Physics, University of Hyderabad, Hyderabad – 500046, India*
[a]*Corresponding author: satishayila@rguktn.ac.in*

**Abstract.** The superparamagnetic behavior of $Ni_{50}Mn_{29}Ga_{21}$alloy has been studied in ribbon form. The crystal structure was observed to change from 7M orthorhombic to monoclinic from bulk to ribbon. Systematic investigations on the magnetic properties on as cast ribbon reveal the presence of superparamagnetic nature. Blocking temperature and in the ribbon was found to be 45 K which evidences the presence of superparamagnetic nature in the ribbons. The average particle size of 8 nm was estimated from the blocking temperature and magnetocrystallineanisotropy constant ($K_{eff}$).

**i0020**

**Exploring Half Metallic Ferromagnetic behavior in Full Heusler Compound $LiBaO_2$ via DFT**

Arti Saxena[1], Aparna Dixit[1], Jisha Annie Abraham[2] and Ramesh Sharma[3]*
*1Department of Basic Sciences and Humanities, Pranveer Singh Institute of Technology, Kanpur, (U.P) India.*
*2Department of Physics, National Defence Academy, Khadakwasla, Pune -411023, (Maharashtra) India*
*3Department of Applied Science, Feroze Gandhi Institute of Engineering and Technology, Raebareli-229001, (U.P) India*
**Email: sharmadft@gmail.com*

Density functional theory employing the generalized gradient approximation has been applied to explore the electronic structure and magnetic characteristics of the $LiBaO_2$ full-Heusler compound. $LiBaO_2$ compounds were predicted to be ferromagnetic half-metals in both the $CuHg_2Ti$ and $Cu_2MnAl$ phases. But findings demonstrated that the $LiBaO_2$ crystallizes in $Cu_2MnAl$-type structure in ferromagnetic phase as its equilibrium ground energy is less in this phase. The spin-polarized computations show that $LiBaO_2$ is a newly developed d0 half-metal that follows the Slater-Pauling rule. The system stabilizes in a ferromagnetic ground state at its equilibrium lattice parameter, yielding a net magnetic moment of 1.0 μB per unit cell. The strong spin polarization present in the oxygen p-states is the main factor driving the material's magnetism and half-metallic properties. The findings demonstrate that $LiBaO_2$ compounds are appropriate for use in spintronics applications.

**i0021**

**Magneto-Optical Kerr Effect of 2D Altermagnetic MnTe: A First-Principles Study**

Nimin K.[#] Alveera[#] and R. Thangavel*
[1]*Semiconductor Research and Device Laboratory, Department of Physics, Indian School of Mines, Dhanbad 826004, Jharkhand, India.*
[#] *Equal contribution of manuscript*
[*]*E-Mail: rthangavel@iitism.ac.in*

We report on the diagonal and off-diagonal components of the optical conductivity revealed strong interband transitions and magneto-optical activity intrinsic to the altermagnetic ordering in Manganese telluride (MnTe). Magneto-optical Kerr rotation ($\theta_k$) and ellipticity ($\eta_k$) spectra exhibit distinct features, with a prominent Kerr rotation peak 0.35° between 0.85–1.45 eV, driven by off-

diagonal conductivity components ($\sigma_{xy}$). These spectra reflect Kramer's–Kronig behavior, with zero-crossings in $\theta_k$ coinciding with extrema in $\eta_k$. The result obtained using magneto-optical response shows the role of symmetry breaking and altermagnetic nature in 2D MnTe. The calculated Magneto-optical Kerr effect (MOKE) results establish MnTe as a strong candidate for spintronic device applications.

**i0022**

**Magnetic and Magneto-functional Properties of Pure and Doped DyGa2 Alloys**

Anirban Saha*, Sanchita Ghosh, Sanat Kumar Adhikari, Riya Roy, and Souvik Chatterjee
*UGC-DAE Consortium for Scientific Research, Kolkata Centre, Sector III, LB-8, Salt Lake, Kolkata 700 106, India.*
**Email: anirbansaha834@gmail.com (Email of corresponding author)*

A comparative study of structural, magnetic, and magnetocaloric behavior of polycrystalline antiferromagnetic $DyGa_2$ alloy and its doped compounds is presented in this report. Room temperature X-ray powder diffraction pattern confirms the pure hexagonal structure with *P6/mmm* space group for all the studied alloys. DC magnetization study reveals an antiferromagnetic (AFM) transition at Néel temperature ($T_N$) around ~ 8-10 K, along with a field-induced AFM to ferromagnetic (FM) transition observed in the alloys below their $T_N$. An intriguing interplay of positive and negative magnetocaloric effect is observed near the phase transition within the pure and doped alloys, which indicates promising potential application for the magnetic refrigeration technique in the cryogenic region.

**i0023**

**Direction Dependent Magnetic and Transport Properties of Czochralski Grown $Co_2FeSi$ Single Crystals**

Manisha Srivastava*, Yash Tijare, Gourav Dwari, Shovan Dan, Ruta Kulkarni, and Arumugam Thamizhavel
*Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research Mumbai, Homi Bhabha Road, Colaba, Mumbai, Maharashtra – 400005, India.*
**Email: manisha.srivastava.res@gmail.com*

We have grown a single crystal of $Co_2FeSi$ using the Czochralski method, in a tetra-arc furnace. We have performed the structural analysis using x-ray diffraction studies and confirmed its face centred cubic crystal structure. From the Laue diffraction studies, we confirmed the good quality of the grown single crystal. We have performed a detailed study on the electrical transport and magnetization studies. The crystals demonstrate a large value of saturation magnetization of 5.80 $\mu_B$/f.u. combined with a low remanence of about 0.35 $\mu_B$/f.u. and a coercivity of about 70 Oe, highlighting their potential for use in spintronic and magnetic device technologies.

**i0024**

**The Effect Of Doping Selenium In $MnBi_2Te_4$ Antiferromagnetic Van Der Waals Layered Material**

N. Kinlekar and K. R. Priolkar
*School of Physical and Applied Sciences, Goa University, Taleigao Plateau, Goa 403206, India*
**krp@unigoa.ac.in*

Tunning spin alignment in antiferromagnetic topological insulator, $MnBi_2Te_4$, was attempted by introducing selenium in place of tellurium. $MnBi_2Te_4$ exhibits a long-range antiferromagnetic ordering with a $T_N$=25 K with a strong out of plane anisotropy. Here, $MnBi_2Te_{4-x}Se_x$ (x=0.6, 0.65, 0.7) show a sharp increase in magnetization at T = 11 K and a broad hump between 130 K-170 K. Though the ferromagnetic like signatures are welcome, these arise due to the formation of Mn doped $Bi_2Te_3$ with MnSe as secondary phase, rather than $MnBi_2Te_{4-x}Se_x$ phase.

**i0025**

**Crystal Electric Field Analysis of $CeRu_2Ge_2$**

Shovan Dan[1,a)], Gourav Dwari[1], Suman Nandi[1], Ruta Kulkarni[1], P.D Babu[2], A. Thamizhavel[1,b)]
*[1]Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai 400005, India*
*[2]UGC DAE Consortium for Scientific Research Mumbai Centre, 246 C,Common Facility Building BARC Campus, Mumbai 400085, India*
*Corresponding authors: [a)]dan.shovan@gmail.com, [b)] thamizh@tifr.res.in*

We report a detailed anisotropic studies on the magnetic properties of $CeRu_2Ge_2$ single crystal grown by the Czochralski method. At low magnetic fields, in addition to the known ferromagnetic transition at $T_C$ = 7.5 K, an additional antiferromagnetic (AFM) anomaly emerges at $T_N$ = 8.1 K. This AFM ordering is highly fragile, being suppressed under higher magnetic fields, and is absent in the specific heat data. The pronounced anisotropy observed in the magnetic susceptibility and magnetization along the [100] and [001] directions is quantitatively explained within the crystal electric field (CEF) framework using the point-charge model. The analysis reveals a CEF level scheme comprising three doublets, with a ground state and excited states at 458 and 593 K.

**i0027**

**Substantial enhancement of Magnetofunctional properties in dual-doped MnNiGe alloy**

Sanchita Ghosh*, Anirban Saha, Riya Roy, Sanat Kumar Adhikari, and Souvik Chatterjee
*UGC-DAE Consortium for Scientific Research, Kolkata Centre, Sector III, LB-8, Salt Lake, Kolkata 700 106, India.*

**Email: sanchitaghosh9377@gmail.com (Email of corresponding author)*
Temperature (*T*)-dependent structural and magnetic analysis is performed on the self-doped MnNiGe alloy, having a significant amount of vacancy at the Ni site, through synchrotron X-ray diffraction (XRD) and magnetic measurements. The presence of a martensitic phase transition (MPT) from the $Ni_2In$-type hexagonal to the TiNiSi-type orthorhombic structure is evident from XRD analysis. The presence of a considerable amount of high-*T* austenite phase below MPT confirms that the MPT is incomplete. The MPT of the polycrystalline sample couples with a magnetic transition, which is from incommensurate antiferromagnetic (AFM) in the martensite to commensurate AFM structure in the austenite phase. On further heating the sample, the austenite phase undergoes another magnetic phase transition from commensurate AFM to a paramagnetic state. Moreover, with increasing applied magnetic fields (*H*), a field-induced transition is observed. Another unique observation is the non-monotonic nature of the inverse magnetocaloric effect. Interestingly, the alloy also shows a spin-reorientation transition in the magnetically ordered austenite phase.

**i0029**

**Structural, magnetic, and electrical properties of $SmAg_2Ge_2$ single crystal**

Kanchan Bala[1a], Suman Nandi[1], Shovan Dan[1], Ruta Kulkarni[1], and Arumugam Thamizhavel [1]
[1]*Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai 400005, India*
[a)]*Corresponding author: kanchan.bala@tifr.res.in*
We report the successful growth of high-quality single crystals of $SmAg_2Ge_2$ using the self-flux method. Phase purity and crystal structure were confirmed by powder X-ray diffraction with Rietveld refinement, and the crystallinity was validated through Laue diffraction patterns. $SmAg_2Ge_2$ crystallizes in the well-known $ThCr_2Si_2$-type tetragonal structure with space group *I4/mmm* (No. 139). Detailed measurements of magnetic susceptibility, electrical resistivity, and heat capacity reveal pronounced anisotropy reflecting the tetragonal crystal structure. The DC magnetic susceptibility, electrical resistivity, and heat capacity measurements indicate that this compound undergoes an antiferromagnetic transition at 9.2 K.

**i0030**

**Effect of Correlation on the Pressure-Induced Insulator to Metal Transition in Double Perovskites**

Vineeta Yadav, Sromona Nandi, and Rudra Sekhar Manna*
*Department of Physics, Indian Institute of Technology Tirupati, Tirupati, Andhra Pradesh 517619, India*
**Email: rudra.manna@iittp.ac.in*
We study the effect of correlation (*U*) for the pressure-driven insulator to metal transition for antiferromagnetic double perovskite oxides using first-principles electronic structure calculations. $La_2CoTiO_6$ (LCTO) shows an antiferromagnetic insulating (AFM-I) ground state whose band gap increases as correlation (*U*) increases. With the application of hydrostatic pressure, the band gap decreases, and for critical pressure, the system transforms to an antiferromagnetic-metallic (AFM-M) state. Indeed, the value of the critical pressure increases as *U* increases. Compared to its isostructural counterpart $La_2NiTiO_6$ (LNTO), which requires significantly higher pressure for obtaining the similar phase transition, implying LCTO exhibits a more pressure-sensitive gap behavior. These findings highlight the tunability of correlated oxides through pressure and electron correlations, offering insights for materials design.

**i0031**

**Unravelling the Incoherent-Coherent Crossover in Itinerant Ferromagnet $Fe_3GeTe_2$**

Deepali Sharma, Asif Ali, Neeraj Bhatt, Rajeswari Roy Chowdhury, Chandan Patra, Ravi Prakash Singh, and Ravi Shankar Singh[(a)]
*Department of Physics, Indian Institute of Science Education and Research Bhopal, Bhopal Bypass Road, Bhauri, Bhopal – 462066, M. P., India*
**Email: rssingh@iiserb.ac.in*
Two-dimensional (2D) van der Waals ferromagnets offer a versatile platform for both spintronic applications and the investigation of low-dimensional magnetism. $Fe_3GeTe_2$ stands out for its complex interplay of localized and itinerant electronic states. We investigate the temperature dependent electronic structure of $Fe_3GeTe_2$ using high-resolution photoemission spectroscopy combined with density functional theory plus dynamical mean-field theory. Our experimental spectra reveal the emergence and evolution of a quasiparticle peak near the Fermi level below 125 K, indicative of an incoherent-to-coherent electronic crossover. Theoretical calculations further support this scenario, with the quasiparticle scattering rate becoming smaller than the thermal energy below ~150 K. These findings provide direct evidence of a temperature-driven coherence transition and role of electronic correlations in $Fe_3GeTe_2$.

**i0032**

**Influence of Loop Current in Kagomé Superconductors**

Pujita Das[1], Tulika Maitra[1], and Narayan Mohanta[1]*
[1]*Department of Physics, Indian Institute of Technology Roorkee, Roorkee 247667, Uttarakhand, India*
**Email: narayan.mohanta@ph.iitr.ac.in*
Motivated by recent breakthroughs in superconductivity and a successive evolution of electronically ordered states in the vanadium-based kagomé-lattice metallic compounds $AV_3Sb_5$ (*A* = K, Rb, Cs), we perform a self-consistent theoretical study on the superconducting properties of the two-dimensional kagomé lattice. Using the Bogoliubov-de Gennes mean-field theory at very low

temperatures, we investigate theoretically the impact of the orbital loop current on the superconducting properties. It is revealed that superconductivity in the kagomé lattice diminishes as the orbital loop current amplitude grows, due to its interplay with charge order and orbital loop current. In addition, when subjected to a Zeeman magnetic field, the presence of charge order, intertwined with the time-reversal symmetry breaking orbital loop current, can deform the U-shaped, fully gapped density of states into a pseudo-gap V-shaped density of states.

**i0033**

**Magneto-structural Coupling in the Layered Honeycomb Lattice Compound $Na_2Co_2TeO_6$**

Anjali Kumari,[1,2] Aprajita Joshi,[3] Surajit Saha,[3] A. K. Bera[1,2 a)], S. M. Yusuf[1,2]
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*
[3]*Department of Physics, Indian Institute of Science Education and Research, Bhopal 462066, India*
**akbera@barc.gov.in (Email of corresponding author)*

The two-dimensional layered honeycomb antiferromagnet $Na_2Co_2TeO_6$ (NCTO), a promising candidate for hosting Kitaev quantum spin liquid states, exhibits a complex magnetic phase diagram in the H-T plane with magnetic ordered and disordered states. However, the interplay between its spin, lattice, and electronic degrees of freedom remains unresolved. Here, we employ temperature-dependent Raman spectroscopy together with single crystal magnetization measurement to probe NCTO's magneto-structural coupling. Our study reveals distinct signatures of spin-phonon coupling at the three temperature dependent magnetic phase transition temperatures at 17, 27, and 130 K in zero field. Furthermore, we identify appearance of additional Raman mode below the ferroelectric ordering temperature at 80 K, arising from its non-centrosymmetric structure, suggesting a coupled magneto-electric effect. These findings highlight the role of magneto-structural coupling on the emergent quantum magnetism and multiferroicity in NCTO.

**i0034**

**Electronic Structure Study of Hole Doped $La_2NiO_4$**

Haritima Mahajan, Deepali Sharma, Neeraj Bhatt, and Ravi Shankar Singh[(a)]
*Department of Physics, Indian Institute of Science Education and Research Bhopal,*
*Bhopal Bypass Road, Bhauri, Bhopal – 462066, M. P., India*
**Email:rssingh@iiserb.ac.in*

The recent discovery of unconventional superconductivity in layered nickelates has sparked renewed interest in their magnetic and electronic properties. The magnetic configurations of layered nickelates at ambient pressure, strongly associated with spin-charge fluctuations, remain a subject of debate. In this work, we investigate the evolution of electronic and magnetic structure in a hole-doped single-layer nickelate, $La_{2-x}Sr_xNiO_4$ ($x$ = 0, 0.33, 0.5, 0.67), using density functional theory (DFT). Our findings reveal a lower density of states at the Fermi level, predominantly driven by the Ni 3*d* states, indicating metallic behaviour. The ground state for the undoped system is found to be an antiferromagnetic insulator, while doped compounds are found to be antiferromagnetic metals. A comparison of the DFT and DFT+*U* results highlights the role of strong electron correlation in the electronic structure of single layer nickelates.

**i0035**

**The Frustration-Driven Magnetism and Glassy Dynamics in Spin-Chain Compound $Ca_3Co_2O_6$**

Priyanka S. Mahalle[1,2], A. Kumar[1,2 a)], S. Saini[3], and S. M. Yusuf[1,2]
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai-400085*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai-400094*
[3]*Materials Science Division, Bhabha Atomic Research Centre, Mumbai- 400085*
[a)] *Corresponding author: amitkr@barc.gov.in*

$Ca_3Co_2O_6$ is a quasi-one-dimensional spin-chain oxide exhibiting exotic magnetic order and pronounced geometrical frustration. In this work, we present a comprehensive investigation of its crystal and magnetic structure utilizing neutron powder diffraction (NPD), X-ray diffraction, and detailed magnetization measurements. Our NPD study reveals the emergence of a modulated, partially disordered antiferromagnetic (PDA) structure at 24 K, along with the coexistence of short-range magnetic ordering at low temperatures (> 10 K). DC magnetization studies corroborate these findings, while AC susceptibility measurements demonstrate slow spin dynamics and strong frequency-dependent behaviour, indicative of glassy magnetic freezing and dynamical frustration. Altogether, these findings present the intricate interplay between lattice geometry, spin anisotropy, and magnetic frustration in this low-dimensional cobalt oxide.

**i0036**

**Engineering Ferromagnetism in Wide Band Gap w-AlN for Spintronic Applications: Insights from DFT Calculations**

Chinnappan Ravi
*Materials Modeling Section, Defects and Damage Studies Division, Materials Science Group, Homi Bhabha National Institute, Kalpakkam 603102, Tamil Nadu, India*
*Email:ravic@igcar.gov.in*

Spintronics, with its promise of enhanced data storage and quantum computing, hinges on the development of practical dilute magnetic semiconductors (DMS). This presentation details a theoretical investigation into the magnetic properties of Cr, Ru, and Rh-doped w-AlN, using spin-polarized density functional theory (DFT) calculations with supercell models. Analysis of our formation energies of point-defects reveals that $Cr^{4+}$, $Ru^{4+}$, and $Rh^{3+}$ are the most probable charge states for these dopant atoms substituting Al in w-AlN. Significantly, Cr-doped AlN demonstrates stability in the ferromagnetic state, crucial for spintronic devices, across a range of Cr concentrations (1.85 to 16.67% of Al). Conversely, Ru and Rh-doped AlN, even in their preferred charge state, were found to be unstable in the ferromagnetic configuration. Further investigation into the electronic density of states (DOS) of ferromagnetic Cr-doped AlN highlights a fascinating evolution: it remains insulating for Cr concentrations below 5.56%, transitions to a half-metal state between 7.40 and 12.96%, and finally becomes a normal metal at 16.67% Cr. This tunable electronic behavior, particularly the half-metallic characteristic, is absent in the energy-favored antiferromagnetic states of Ru and Rh-doped systems. This work provides crucial theoretical insights into engineering ferromagnetic w-AlN, a promising material for future spintronic technologies.

**i0037**

**Novel Synthesis and Magnetic Characterization Of Skyrmion Host Polycrystalline Multiferroic $Cu_2OSeO_3$**

Remya Krishnan[1], P. D. Babu[2], P.V. Prakash Madduri [1, a)]
[1]*Department of Sciences, Indian Institute of Information Technology Design and Manufacturing Kurnool, Kurnool-518008, Andhra Pradesh, India.*
[2]*UGC-DAE Consortium for Scientific Research, Mumbai Centre, BARC Campus, Mumbai 400 085, India*
[a)]*Corresponding author: prakash.madduri@iiitk.ac.in*

Here, we report a novel gel synthesis technique for preparing skyrmion host multiferroic insulator system $Cu_2OSeO_3$ (CSO) in the polycrystalline form by single-time annealing of $CuSeO_3.2H_2O$, which is prepared from copper nitrate trihydrate ($Cu(NO_3)_2.3H_2O$) and Seleneous acid ($H_2SeO_3$). This technique is feasible as it is comparatively simple and low-power-consuming compared to other solid-state reactions and chemical vapour transport techniques. Thermogravimetric data analysis on $CuSeO_3.2H_2O$, enabled to optimize the formation of $Cu_2OSeO_3$ with an annealing temperature of 475 °C, an annealing time of 24 h, and subsequent cold-water quenching. Structural characterizations confirmed the single-phase nature of $Cu_2OSeO_3$. Thermomagnetic curves yield a transition temperature of 59.50 ± 5 K, which perfectly matches the reported data in the literature. The field-dependent ac susceptibility on the system revealed an extended skyrmion phase over a temperature range of ~8 K below the transition temperature.

**i0038**

**DFT +DMFT Study Of Magnetism In $SrCoO_3$**

Jyotsana Sharma[1,2,a)], Shivani Bhardwaj[1] and Sudhir K. Pandey[3]
[1]*School of Physical Sciences, Indian Institute of Technology Mandi, Kamand - 175075, India*
[2]*Swami Vivekanand Govt. College Ghumarwin - 174021, India*
[3] *School of Mechanical and Materials Engineering, Indian Institute of Technology Mandi, Kamand - 175075, India*
[a)]*Email: jyotsana.sharma1290@gmail.com*

This work presents Density Functional Theory(DFT)-cum-Dynamical Mean Field Theory(DMFT) study of cubic pervoskite SrCoO3. We have used PBEsol exchange correlational functional which gives lattice constant quite close to the experimental values. The momentum-resolved spectral function plot suggests that electronic correlation among Co-d electrons has introduced incoherent states majorly contributed by $t_{2g}$ -dn states. We also investigated quasiparticle lifetime and $Im\Sigma(\omega)$ to confirm Fermi-Liquid behaviour. The Hubbard parameters $U_{full}$ = 4.80 eV and $J_{crpa}$ = 0.72 eV obtained using constrained Random Phase Approximation gave Tc ~ 300K in fair agreement with the experimental results.

**i0039**

**Length-Dependent Localization of Majorana Bound States in Rashba and Magnetically Textured Nanowires**

Pankaj Sharma* and Narayan Mohanta
*Department of Physics, Indian Institute of Technology Roorkee, Roorkee, India 247667*
**pankaj@ph.iitr.ac.in*

We study the spatial localization of Majorana bound states in finite one-dimensional nanowires with effective p-wave superconductivity induced via Rashba spin–orbit coupling, Zeeman field, and proximity-induced s-wave pairing. Additionally, we explore an analogous system without any external magnetic fields by introducing engineered spin-spiral textures that replicate the effects of Rashba spin-orbit coupling and Zeeman field. By computing the local density of states of the two zero-energy quasiparticle eigenstates as a function of wire length, we identify two critical length scales, $L_{c1}$ and $L_{c2}$, which mark the distinct regimes of localization of Majorana bound states. For $< L_{c1}$, the states are strongly hybridized, contributing equally at both ends. For $L_{c2} < L$, each state is localized at a separate end, consistent with ideal end-localized Majorana bound states. The intermediate regime ($L_{c1} < L < L_{c2}$) exhibits partial localization with residual overlap. Notably, the crossover occurs at a shorter length in spin-textured nanowires, suggesting stronger Majorana bound states confinement than in Rashba-based systems. These findings provide insight into how finite-size effects govern the emergence and spatial separation of Majorana bound states in realistic platforms.

**i0040**

**Magnetic Anisotropy In Self-Organized Fe Nanostructures Fabricated Through Impurity-Assisted Surface Nanopatterning**

Amruta A[1], Anup Kumar Bera[2], Sarathlal Koyiloth Vayalil[3], Benedikt Sochor[3], Dileep Kumar[1,a]
[1] *UGC-DAE Consortium for Scientific Research, Khandwa road, Indore, Madhya Pradesh – 452001*
[2]*Department of Materials Engineering, CV Raman Road, IISc, Bangalore -560012*
[3]*Deutsches Elektronen-Synchrotron DESY, Hamburg 22607, Germany*
[a)] *Corresponding author email: dkumar@csr.res.in*

We present a detailed investigation of Fe nanostructures formed on Si(001) substrates using ion beam erosion deposition (IBED), a technique that combines simultaneous ion irradiation and metal incorporation during film growth. In this study, the sample was synthesized under oblique $Ar^+$ ion irradiation at a 20° incidence angle, enabling self-organized ripple morphology to emerge through impurity-assisted surface patterning. Structural and magnetic characterizations were performed using X-ray reflectivity (XRR), grazing incidence small-angle X-ray scattering (GISAXS), grazing incidence wide-angle X-ray scattering (GIWAXS), atomic force microscopy (AFM), and magneto-optical Kerr effect (MOKE). XRR revealed a ~1.7 nm film with moderate roughness, and GISAXS showed asymmetric scattering indicative of inclined ripple structures. GIWAXS confirmed a polycrystalline Fe phase with a tilted (110) texture. AFM and height–height correlation function (HHCF) indicated grain alignment with a correlation length of ~113 nm. MOKE loops revealed uniaxial magnetic anisotropy with the easy axis perpendicular to the ion beam. Although polycrystalline Fe films do not typically exhibit strong magnetic anisotropy, our results demonstrate that the IBED approach can induce and tune UMA by tailoring the surface morphology and local structure. These findings highlight the capability of IBED to induce coupled morphological and magnetic anisotropy, making it a valuable tool for nanoscale magnetic engineering.

**i0041**

**Thickness-dependent Exchange Bias In Polycrystalline $Fe_3O_4$ Thin Films: Interfacial Coupling With FeO And Cooling Field Effects**

Aritra Ray[1] and Perumal Alagarsamy[1a]
[1]*Department of Physics, Indian Institute of Technology Guwahati, Assam 781039, India*
[a]*Corresponding author: perumal@iitg.ac.in*

Exchange bias (EB) in single-layer films has emerged as a key feature for advancing spintronic technologies, yet its origin in such systems remains less understood. Our study revealed a significant EB field of 550 Oe observed in 30 nm films of $Fe_3O_4$/Si(100) under field-cooling, while temperature- and field-dependent magnetization investigations indicated the presence of antiferromagnetic FeO in the same film. Meanwhile, Structural analysis confirms single-phase polycrystalline $Fe_3O_4$ with increasing surface roughness at higher thicknesses. The magnetization anomalies linked to the FeO diminished with increasing film thickness owing to the reduced volume fraction of the FeO, as confirmed through XPS analysis. Remarkably, a zero-field cooled EB was observed for the thinner films caused by the development of anisotropy due to strong interfacial exchange coupling at the $Fe_3O_4$/FeO interface, which can be dramatically tuned by a cooling field. The tunability of EB via film thickness and cooling field highlights the potential application of single-layer ferromagnetic $Fe_3O_4$ films, allowing precise control over pinning dynamics of the reference layer in MRAM devices.

**i0044**

**Low Magnetic Moment and Negative Magnetoresistance in Inverse Heusler Alloy-$Cr_2CoAl$**

Aparna Ashok, Neeru Bhagat
*Department of Applied Science, Symbiosis Institute of Technology, Symbiosis International (Deemed) University, Pune, Maharashtra, 412115, India*
**aparna007ashok@gmail.com*

Heusler alloys find their applications as sensors, actuators, energy harvesters, and as magnetic cooling devices. Negative magnetoresistance (NMR) in inverse Heusler compounds is a fascinating phenomenon that has attracted significant attention due to its potential applications in spintronics and magnetic device technology. In these compounds, NMR arises from the unique electronic and magnetic properties of the material's crystal structure and electronic band structure. In the inverse Heusler compound Cr2CoAl, Cr and Co are transition metals, and Al is the main group element. Studies on temperature-dependent magnetization (M-T) under zero-field cooled (ZFC) and field cooled (FC) conditions as well as field-dependent magnetization (M-H) between a temperature range of 5-300 K suggest that this compound has a very low magnetic moment. The resulting reduction of magnetic moment and NMR is due to the compensation of the moments carried by the different sublattices.

**i0045**

**Mn Doping Effects on Structural and Magnetic Properties of $NiFe_2O_4$ Nano-Ferrites**

Shravya Borkar[1], Joshle Colaco[1], Kimberly Estibeiro[1], Chloy Costa[1], Yatin P. Desai[1, a)] and Manoj M. Kothawale[2]
[1]*Department of Physics, CES's Parvatibai Chowgule College of Arts and Science, Autonomous, Margao Goa, 403602, India*
[2]*Department of Physics, Dnyanprassarak Mandal's College, and Research Centre, Assagao – Goa, 403 507, India*
[a)]*Corresponding author: ypd001@chowgules.ac.in*

Mn-doped nickel ferrite nanoparticles with the formula $Ni_{1-x}Mn_xFe_2O_4$ (x = 0.0, 0.2, 0.4, 0.6, 0.8) were synthesized using the sol-gel auto-combustion method. X-ray diffraction study confirmed a cubic spinel structure, with the lattice parameter increasing systematically with $Mn^{2+}$ content. SEM images revealed spherical nano-sized particles with slight agglomeration. Saturation magnetization (Ms) measured by SQUID varied from 25.55 to 44.26 emu/g, and all samples showed low coercivity, confirming

their soft magnetic nature. The composition-dependent variations in structural and magnetic properties make these ferrites attractive for soft magnetic applications.

**i0046**

**First-Principles Study of Altermagnetism in $MnF_2$**

Rupam Tamang,[1, 2,] D. Gurung[1], Shivraj Gurung[2], D. P. Rai[1, a)], Keshav Shrestha[3], Shalika R. Bhandari[4], Samy Brahimi[5,6], Samir Lounis[6]

[1]*Department of Physics, Mizoram University, Aizawl-796004, India*

[2]*Physical Sciences Research Center (PSRC), Department of Physics, Pachhunga University College, Aizawl-796001, India*

[3]*Department of Chemistry and Physics, West Texas A&M University, Canyon, Texas 79016, USA*

[4]*Department of Physics, Bhairahawa Multiple Campus, Tribhuvan University, Nepal*

[5]*Laboratoire de Physique et Chimie Quantique, Universite Mouloud Mammeri de Tizi-Ouzou, 15000 Tizi-Ouzou, Algeria*

[6]*Institute of Physics, Martin-Luther-University Halle-Wittenberg, 06099 Halle (Saale), Germany*

[a)]*Corresponding author: dibyaprakashrai@gmail.com*

In this article, we explore altermagnetism in the insulating altermagnet candidate $MnF_2$ using density functional theory (DFT). Within the GGA+U formalism, we find the highest non-relativistic spin splitting (NRSS) of ~273 meV and ~225 meV in the conduction and valence bands, respectively. The presence of spin-polarized band structures without SOC supports $MnF_2$ as a potential altermagnet. The direct-space magnetization density shows an anisotropy between spin-up and spin-down channels, complementing the altermagnetic order in this material. Incorporating relativistic SOC in the GGA+U calculation, we compute magneto-transport properties through maximally localized Wannier functions (MLWFs). The calculated value of the spin Hall conductivity peaks in the conduction band, reaching approximately $153(\frac{\hbar}{e}\,\mathrm{S\cdot cm^{-1}})$.

**i0047**

**Effects of Quenched Disorder on Pair Density Wave**

Shashwat Chaturvedi* and Peayush Kumar Choubey

*Department of Physics, Indian Institute of Technology Roorkee, Roorkee 247667, Uttarakhand, India.*

**Email: shashwat_c@ph.iitr.ac.in*

We study the emergence of pair density wave (PDW) order in a microscopic model with pair-hopping interaction by employing a self-consistent real-space Bogoliubov-de Gennes (BdG) approach. For a wide range of model parameters, we find a stable PDW ground state accompanied by an induced CDW, which was ignored in previous momentum-space-based studies. We investigate the effects of a single impurity on the local electronic structure and extend our analysis to systems with multiple impurities. Our results would highlight the sensitivity of PDW to disorder.

**i0048**

**Two-Step Field-Induced Spin-Flip Metamagnetic Transitions in the Novel Tellurate Compound $Na_4NiTeO_6$**

Shubham Patil and S. D. Kaushik

*UGC-DAE Consortium for Scientific Research Mumbai Centre, Bhabha Atomic Research Centre, Mumbai, 400085, India*

** shubham@csr.res.in*

We report the synthesis and comprehensive characterization of stoichiometric $Na_4NiTeO_6$, a quasi-one-dimensional spin-chain compound. Structural refinement using X-ray and neutron powder diffraction confirms a layered structure comprising edge-sharing $NiO_6$ octahedra forming zigzag chains along the a-axis. The temperature-dependent DC magnetic susceptibility reveals a transition to a magnetically ordered state at $T_N \approx 7$ K. Curie-Weiss analysis indicates dominant ferromagnetic interactions and an enhanced effective moment of 3.21 $\mu_B$ per $Ni^{2+}$. Isothermal magnetization data show two-step spin-flip transitions at 2.5 K, suggesting field-induced metamagnetic behavior and magnetic anisotropy. The observed phenomena likely arise from competing intra and inter-chain interactions in the quasi-1D lattice. These findings position $Na_4NiTeO_6$ as a promising candidate for studying low-dimensional quantum magnetism and frustration. Ongoing neutron scattering studies aim to elucidate its magnetic ground state and exchange pathways.

**i0049**

**Temperature Dependent Terahertz Spectroscopy of Mg doped NiO**

Anushka Kshirsagar;[1a)], Anol Mondal[1], Sudeep Tiwari[1b)] and S.S.Prabhu[1]

[1]*Tata Institute of Fundamental Research, Mumbai,400005, India*

*Corresponding author email: [a)] anu.kshirsagar.231@gmail.com [b)] sudeep.tiwari@tifr.res.in*

$Mg_{.05}Ni_{0.95}O$ nanoparticles (MNO NPs) were prepared via the sol-gel technique, exhibiting a particle size of approximately 44 nm. These nanoparticles crystallized in a single-phase face-centered cubic (fcc) symmetry (space group: Fm-3m No. 225). Temperature-dependent magnetization studies of MNO NPs reveal weak ferromagnetic-like behaviour, attributed to uncompensated surface effects. Terahertz Time Domain Spectroscopy (THz-TDS) was employed to explore the optical properties of these nanoparticles. The refractive index (n) ranged from 2.25 to 2.30 across the temperature range of 16 K to 300 K, while the extinction coefficient (k) followed a similar trend to that of n. Dielectric parameters derived from THz-TDS suggest that MNO NPs serve as effective insulators of the THz electric field at lower temperatures.

**i0050**

**Magnetic Properties of Kagome Magnet $DyCo_3$**

Bhagyashree Pol*, Anu and P. D. Babu
*UGC-DAE Consortium for Scientific Research, Mumbai Centre, BARC Campus, Mumbai- 400085, India*
*shreepol@csr.res.in

The Kagome magnet $DyCo_3$, was investigated using dc-magnetization and heat capacity measurements as function of temperature and magnetic field. The compound crystallizes in rhombohedral structure with $R\bar{3}m$ space group. The dc magnetization data indicate magnetic transition at ~ 450 K and ZFC curve goes negative moment side with a compensation temperature of 47 K. Magnetic isotherms show metamagnetic transition that is signature of AFM to FM transition for temperatures below 50 K that is characteristic of non-collinear magnetic systems. Magnetization saturate in high field with finite coercivity. Energy barrier for pinning domain wall α is ~280.5 μeV. The value of Sommerfeld coefficient and Debye temperature is 46.9 mJ/mol-$K^2$ and $\theta_D$ is ~ 209 K respectively. Results indicate complex magnetic structure in this compound.

**i0052**

**Design, Green Synthesis, Magnetic Characterization and Biological Evaluation of Mg and Ca Doped Zn-Co Nanoferrites**

Anisha Bano[1*], Manisha[1], Sudeep Tiwari[1], S. S. Meena[2], Prashant B. Kharat[3], Pratik Pramod Shinde[4], Anupama Mittal[5] and Sudhish Kumar[1]
[1]*Magnetism Laboratory, Department of Physics, Mohanlal Sukhadia University, Udaipur -313002, India*
[2]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, India*
[3]*Department of Physics, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad-431004, India*
[4]*Department of Pharmacy, Birla Institute of Technology & Science, Pilani-333031, India*
[5]*Department of Pharmaceutics, NIPER, SAS Nagar, Punjab-160062, India*
**Email: anishabano687@gmail.com*

In recent years, spinel structured nanoferrite particles (NFPs) have caught significant attention due to high chemical stability, excellent magnetic properties and lot of promise for the magnetic hyperthermia based safer cancer treatments. Here, we report the effect of Mg and Ca doping on the magnetic properties, heating efficiency and biological evaluation of $Zn_{0.5}Co_{0.5}Fe_2O_4$ (ZCF5), $Zn_{0.5}Co_{0.5}Fe_{1.8}Mg_{0.2}O_4$ (ZCFM) and $Zn_{0.5}Co_{0.5}Fe_{1.8}Ca_{0.2}O_4$ (ZCFC) NFPs prepared via sugarcane juice assisted sol-gel auto-ignition route. PXRD, FTIR and Raman investigations confirmed phase pure formation of these NFPs in the fcc structure (space group $Fd\bar{3}m$). Magnetization and $^{57}Fe$ Mössbauer spectroscopic studies revealed co-existence of dominant superparamagnetic phase and minor soft ferrimagnetic phase at 300 K in these NFPs. Induction heating and *in-vitro* cell analysis indicated superior hyperthermic response and good biocompatibility of these NFPs against human normal cells (HEK293) and lethal response against breast cancer cells (MCF-7). It is worth to note that $Mg^{2+}$ and $Ca^{2+}$ doping in Co-Zn ferrite greatly modifies the magnetic and hyperthermic response with improved biocompatibility.

**i0053**

**Role Of Tm Ions In Modulating Magnetic Damping Of YIG**

Simran Sahoo [1*], Shrawan K. Mishra[1]
[1]*School of Materials Science and Technology, Indian Institute of Technology BHU, Varanasi, India*
**Email: simransahoo.rs.mst23@itbhu.ac.in*

Magnetic garnet thin films offer an unique platform for exploring low-damping spin dynamics, positioning them as key materials in modern spintronics and magnonics. Yttrium iron garnet (YIG) is well-known for its exceptional electrical and magnetic properties. They possess promising properties like superior thermal and chemical stability, high Curie temperatures, and low magnetic damping. The substitution of thulium (Tm) into yttrium iron garnet (YIG) thin films introduces significant modifications to their magnetic dynamic properties, making them promising candidates for tunable spintronic and magnonic applications. In this study, we investigate the effects of $Tm^{3+}$ ion incorporation on key magnetic parameters such as Gilbert damping, ferromagnetic resonance (FMR) linewidth, and magnetic anisotropy. A comparative study of different percentage Tm doped YIG has been done to see how the parameters like saturation magnetization and damping parameter evolve. Angle dependent FMR study has been done to see the magnetic anisotropy. These findings provide crucial insights into engineering i.e the magnetic relaxation mechanisms in garnet-based thin films, with implications for the design of high-frequency, low-power magnetic devices.

**i0054**

**Field induced spin freezing and Schottky anomaly in $Gd_2Hf_2O_7$ pyrochlore**

Sujata [1, a)] and C. S. Yadav [1, b)]
[1]*School of Physical Science, Indian Institute of Technology Mandi, Kamand, Mandi, HP 175005*
[a)] *Email: d22157@students.iitmandi.ac.in*
[b)] *Email: shekhar@iitmandi.ac.in*

Spin ice materials serve as exemplary systems that exhibit zero-point entropy as their temperature approaches absolute zero, resulting from their disordered configurations [1,2]. Hafnate compounds with pyrochlore structure ($A_2Hf_2O_7$, where A represents a rare earth ion and O is oxygen) consist of corner-sharing tetrahedra. The magnetic ions located at the vertices of these tetrahedra give rise to exotic magnetic states [3,4]. we investigate the structural and magnetic properties of disordered polycrystalline

pyrochlore $Gd_2Hf_2O_7$ compound. The magnetic heat capacity reveals antiferromagnetic short-range interactions ($J_{nn}$ = -0.19 K, $D_{nn}$ = 1.26 K) at low temperatures, which are completely suppressed under at 3 T field. We performed a comprehensive analysis of magnetization to understand the evolution of spin dynamics at low temperatures in the presence of an external magnetic field (0 - 70 KOe). The isothermal magnetization M(H) curve at 2 K shows a tendency toward saturation, with an effective magnetic moment reaching approximately 7 $\mu_B/Gd^{3+}$ for the free ion $^8S_{7/2}$ ground state of $Gd^{3+}$. The magnetic entropy in zero field reaches Rln8 which is almost equal to total spin entropy. These results suggest the absence of single-ion anisotropy in $Gd^{3+}$ [5].

**i0055**

**Magnetic and Superconducting Properties of $V_{0.99-X}Ti_XGd_{0.01}$ Alloys**

Asi Khandelwal[1, 2, a)], L.S. Sharath Chandra[1, 2, b)], Archna Sagdeo[2, 3, c)] and M.K. Chattopadhyay[1,2, d)]
[1]*Free Electron Laser Utilization Laboratory, Raja Ramanna Centre for Advanced Technology, Indore, Madhya Pradesh - 452 013, India*
[2]*Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400 094, India*
[3]*Accelerator Physics and Synchrotrons Utilization Division, Raja Ramanna Centre for Advanced Technology, Indore, Madhya Pradesh - 452 013, India*
**Email: asikhandelwal1503@gmail.com*

We report studies on the temperature and magnetic field dependence of $V_{0.99-X}Ti_XGd_{0.01}$ alloy superconductors. With increasing Ti content in the $V_{0.99-X}Ti_XGd_{0.01}$ alloys, the superconducting transition temperature ($T_c$), critical current density ($J_c$), and irreversibility field ($H_{irr}$) all show a significant improvement. The $T_c$ enhancement is attributed to the suppression of itinerant spin fluctuations upon substituting V with Ti in the V–Ti alloys. The field up to which $J_c$ persists also increases with increasing Ti content. Moreover, magnetization measurements indicate the coexistence of superconductivity and ferromagnetism in these alloys. The temperature dependence of magnetization also indicates flux compression occurring near the $T_c$ of the alloys.

**i0056**

**Structural and Magnetic Study of High Entropy Spinel Oxide with Five Cations at Both Sublattice**

Rohan Kamble[1, 2, a)], Smita Borole[1, 2], Nilofar Kurawle[1, 2], and Sudhindra Rayaprol[1, 2]
[1]*UGC-DAE Consortium for Scientific Research, Mumbai Centre, BARC Campus, Mumbai- 400085, India.*
[2]*Savitribai Phule Pune University, Ganeshkhind, Pune - 411007, India.*
[a)] *rohank@csr.res.in*

A high-entropy spinel oxide $(Mg_{0.2}Co_{0.2}Ni_{0.2}Cu_{0.2}Zn_{0.2})(Cr_{0.4}Mn_{0.4}Fe_{0.4}Al_{0.4}Ga_{0.4})O_4$ was synthesized via the conventional solid-state route. X-ray and neutron powder diffraction analyses confirmed a single-phase cubic spinel structure ($Fd\bar{3}m$) with site-selective cation distribution, where divalent cations occupy tetrahedral sites and trivalent cations occupy octahedral sites. Magnetic measurements revealed pronounced bifurcation between ZFC and FCW curves, along with negative magnetization in the ZFC branch, indicative of magnetic compensation effects. The ordering temperature was determined to be ~ 104 K from the derivative of magnetization. Isothermal magnetization at 5 K exhibited significant coercivity (~ 2 kOe) and remanence (~ 13 emu/g), and absence of saturation up to 90 kOe. The results highlight the interplay of configurational entropy, and competing magnetic interactions in governing the magnetic behavior of multi-cation spinel oxides.

**i0057**

**Heat Capacity Of $Ho_2Sn_2O_7$ Pyrochlore At Low Temperatures**

Shruti Vyas[1 a)], Manju Mishra Patidar[2,3], R Venkatesh[2], P Saravanan[2], V Ganesan[1]
[1] *Medicaps University, AB Road, Pigdamber, Rau, Indore (MP) 453331, India*
[2] *UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore (MP) 452001, India*
[3] *Presently at Emerald Heights International School, A.B. Road, Rau, Indore (MP) 453331, Indore, India*
[a]*Email:shrutivyas677@gmail.com*

$Ho_2Sn_2O_7$ is a rare earth pyrochlore compound known for its geometrically frustrated magnetic interaction which gives rise to exotic ground states such as spin ice. Sample is prepared using solid state reaction. X-ray diffraction confirmed the phase formation of pyrochlore structure. We have investigated the heat capacity of $Ho_2Sn_2O_7$ down to 2K and magnetic fields up to 3T. Debye contribution to heat capacity has been estimated and the Debye temperature is found to be 354K. The phonon contribution subtracted to get magnetic contribution. This magnetic contribution is typical of Schottky anomaly as there is no tangible magnetic ordering seen down to 2K. This demands ultralow temperature investigation below 2K, which is being planned. Magnetization measurements (not shown here) performed from 2K up to 30K shows no ordering. Hence this sample shows all needy precursor state for a spin ice compound. Results will be discussed.
Keywords- Frustration, Spin ice, pyrochlore

**i0058**

**Influence Of Strontium Doping On The Heat Capacity Properties Of $CuCrO_2$ Delafossite**

Ratnawali Verma[1], Nitu Katariya[2],R. Venkatesh[3], L.S. Sharath Chandra[4],V.Ganesan[1]
[1]*Medi-Caps University, AB Road, Pigdamber, Rau, Indore-45333, MP, India*
[2]*Shri Vaishnav VidhyapeethVishwavidhyalay, Indore-453111, MP, India*
[3]*UGC-DAE Consortium for Scientific Research,Indore-452001, MP, India*

[4]*FEL Utilization Laboratory, Raja RamannaCentrefor Advanced Technology, Indore-452013,MP, India*
** Corresponding author's email address: ratnawaliverma10@gmail.com*
$CuCrO_2$, a prominent delafossite oxide with a layered rhombohedral crystal structure (space group R-3m), exhibits fascinating thermodynamic behavior and potential for electronic applications. In this study, the impact of 5% Strontium (Sr) doping on the structural, optical, thermal and magnetic properties of $CuCrO_2$ was systematically investigated. X-ray diffraction analysis confirmed the rhombohedral structure upon doping, indicating successful incorporation of Sr into the lattice. Low-temperature specific heat measurements, performed using a Physical Property Measurement System (PPMS) under varying magnetic fields, revealed that the antiferromagnetic transition temperature (~24.5 K) of pristine $CuCrO_2$ is suppressed upon 5% Sr doping (23.5). Even though this shift is small, it provide insight into the role of Sr substitution in modifying the thermodynamic behavior of $CuCrO_2$, with implications for tuning its functional properties.

**i0059**

**Magnetization and Heat Capacity of $Co_{0.5}Zn_{0.5}Cr_2O_4$**

Rupali Joshi[1,*], Priya Yadav[1], Malyaj Das[1], Tarun Garg[1], Anand Yadav[1,2], R Venkatesh[3], S D Kaushik[4], P D Babu[4], L S Sharat Chandra[5,6], V Ganesan[1]
[1]*Medi-Caps University, AB Road, Pigdamber, Rau, Indore (MP) 453331*
[2]*Presently at State Forensic Science Laboratory, MPSH 15A, Gopal Ganj, Sagar 470003, India*
[3]*UGC-DAE CSR, IC, University Campus, Khandwa Road, Indore-452001, India*
[4]*UGC-DAE CSR, MC, 246C 2nd Floor, Common Facility Building, BARC Campus, Trombay, Mumbai – 400085, India*
[5]*Free Electron Laser Utilization Laboratory, Raja Ramanna Centre for Advanced Technology, Indore 452 013, India.*
[6]*Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400 094, India.*
**Email: rupali.joshi499@gmail.com*
The substitution of non-magnetic Zn ion on the magnetic Co ion in CoCr2O4 significantly modifies the thermodynamic and magnetic properties of the system. In this research we are focusing on its low temperature heat capacity measurements and temperature dependent magnetic measurement to explain the phase transitions. Specifically, we study the doping affect in magnetic and thermal changes in $Co_{0.5}Zn_{0.5}Cr_2O_4$. . Heat capacity measurements displayed characteristics anomalies at, $T_C$=26K. The study highlights the complex thermodynamical behaviour of zinc-doped cobalt chromite and a role of A-site nonmagnetic ion substitutions in tuning their thermodynamical properties.

**i0062**

**Condensate Pairing Mechanism in Superconducting 6R-$SnNbSe_2$**

K Yadav [1, a)], M Lamba [1)], S Patnaik [1)]
*School of Physical Sciences, Jawaharlal Nehru University, New Delhi-110067, India*
*[a)] Corresponding authors: kunaly51_sps@jnu.ac.ins, spatnaik@jnu.ac.in*
The realization of Majorana fermions, which are fundamental aspects for building fault-tolerant quantum computers, requires materials having superconductivity coexisting with nontrivial band topology. One promising approach is to study topological superconductors (TSCs), which comprise topological materials with broken inversion symmetry. In this study, we report on the synthesis and characterization of a new centrosymmetric material, 6R-$SnNbSe_2$, formed by intercalating Sn atoms into the $NbSe_2$ structure. Using a tunnel diode oscillator technique, magnetic penetration depth and superfluid density down to 1.5 K were measured. The analysis of these measurements indicates that the superconducting state at 4.1 K in 6R-$SnNbSe_2$ has a mix of both nodal and nodeless order parameter symmetry. These unexpected results might be due to the local inversion symmetry breaking in the compound. As a result, 6R-$SnNbSe_2$ serves as an exciting platform for exploring new and unconventional pairing mechanisms in transition metal dichalcogenide superconductors.

**i0063**

**Emergent Magneto-Transport Phenomena in $Ce_2FeAl_3$: Influence of Structural and 4f Electron Correlations**

Nilofar Kurawle[1,2*], Smita Borole[1,2], Rohan Kamble[1,2] and Sudhindra Rayaprol[1,2]
[1]*UGC-DAE Consortium for Scientific Research, Mumbai Centre, CFB-246C, BARC Campus, Trombay, Mumbai – 400085, India*
[2]*Savitribai Phule Pune University, Ganeshkhind, Pune – 411007*
**Email: kurawle31@gmail.com*
$Ce_2FeAl_3$, a ternary intermetallic compound in the Ce–Fe–Al system, exhibits complex magnetic and electronic behavior arising from the interplay between Ce 4f and Fe 3d electrons. Structural analysis confirms a well-ordered cubic crystal structure, providing a symmetric lattice framework conducive to long-range magnetic interactions. Magnetization measurements show a distinct magnetic transition near 280 K, accompanied by irreversibility between zero-field-cooled (ZFC) and field-cooled (FC) curves, indicating magnetic frustration or cluster glass behavior. At low temperatures, $Ce_2FeAl_3$ exhibits strong but unsaturated magnetization up to high fields, suggesting the presence of competing magnetic interactions or partial moment ordering. This behavior is indicative of complex exchange mechanisms, likely governed by a competition between RKKY interactions and Kondo screening of Ce 4f moments. The lack of saturation up to high magnetic fields and bifurcation in ZFC and FC curves may also indicate frustration. These observations point to a magnetically correlated ground state shaped by electron-electron interactions and lattice symmetry. The study highlights the importance of coupling between lattice, spin, and charge degrees of freedom, and sets

the stage for further investigations using techniques such as neutron diffraction to probe the nature of magnetic ordering and the potential emergence of exotic quantum states.

**i0064**

**CoVGe: A low magnetic moment alloy for antiferromagnetic spintronics**

Shoaib Akhtar[1], Jyotiraditya Pandey[1], Ravinder Kumar[1], Samik DuttaGupta[2] and Sachin Gupta[1a]
[1]*Department of Physics, Bennett University, Greater Noida 201310, India*
[2]*CMP Division, Saha Institute of Nuclear Physics, West Bengal, 700064, India*
[a]*Email: sachin.gupta@bennett.edu.in*

The half Heusler alloy CoVGe was synthesized using arc-melt technique and its structural and magnetic properties were investigated. The X-ray diffraction measurements reveal that the material crystallizes in cubic structure with space group $F\bar{4}3m$ and lattice constant 5.81 Å. The magnetic measurements show a Curie temperature of 42 K along with soft-ferromagnetic nature. The total magnetic moment at low temperature and high field was observed to be $0.12\mu_B$ per formula unit. The soft magnetic nature with very low magnetic moment makes this material a promising candidate for antiferromagnetic spintronics.

**i0065**

**Structural, Magnetic and Magneto-caloric effect behaviour of $Ho_2MnCoO_6$**

V R Pooja, A T Sathyanarayana, K. Vinod, and Awadhesh Mani
*Condensed Matter Physics Division, Materials Science Group, Indira Gandhi Centre for Atomic Research, A CI of Homi Bhabha National Institute, Kalpakkam, 603 102, Tamil Nadu, India*
*a) Corresponding author: atsatya@igcar.gov.in*

Polycrystalline $Ho_2MnCoO_6$ synthesized by solid state method has been characterized by X-ray diffraction and magnetization measurements. XRD analysis using Rietveld method indicates the structure as monoclinic with space group $P2_1/n$. Magnetization measurements indicate a ferromagnetic to paramagnetic transition at 81.5 K. Arrot plots discern the transition as second order, though observed nonlinearity in these plots reveal the critical exponents do not belong to universality class of mean field interaction. The system exhibits modest isothermal magnetic entropy change of 5.5 J/kg.K for a field change of 70 kOe.

**i0066**

**Low Temperature Heat Capacity of $NiCr_2O_4$**

Priya Yadav [1*], Rupali Joshi [1], Anand Yadav [1,2], R. Venkatesh[3], L.S. Sharath Chandra [5,6], S D Kaushik[4], P D Babu[4] V. Ganesan [1]
[1] *Medicaps University, AB Road, Pigdamber, Rau, Indore (MP) 453331, India*
[2] *Presently at State Forensic Science Laboratory, MPSH 15A, Gopal Ganj, Sagar 470003, India*
[3] *UGC-DAE CSR, IC, University Campus, Khandwa Road, Indore-452001, India*
[4] *UGC-DAE CSR, MC, 246C 2nd Floor, Common Facility Building, BARC Campus, Trombay, Mumbai – 400085, India*
[5]*Free Electron Laser Utilization Laboratory, Raja Ramanna Centre for Advanced Technology, Indore 452 013, India.*
[6]*Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400 094, India.*
**Email : priyayadav1711@gmail.com*

Nickel chromite ($NiCr_2O_4$) synthesized via the sol-gel method, exhibits a complex interplay of structural and magnetic transitions. The material undergoes a series of structural changes a transition from cubic to tetragonal at 310 K, followed by a second transition from tetragonal to orthorhombic at 65 K, and a third distortion within the orthorhombic structure at 30 K. This complex structural behaviour is coupled with magnetic transitions. At 75 K, the sample transitions from a paramagnetic to a ferrimagnetic state. A further spin re-orientation is observed at 30 K. To understand the low temperature thermal behaviour of the material we perform the heat capacity measurements that confirm these transitions, showing anomalies at these specific temperatures.

**i0067**

**Ferromagnetic Resonance Evidence of Spin Canting in the Spin-Orbit Coupled $4d^3$ Oxide $Ca_3LiRuO_6$**

Babaji Charan Sahoo[1,3,*], Anil Jain[1, 3], S.M. Yusuf[2,3]
[1] *Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, India,*
[2]*Centre of Excellence in Basic Sciences, University of Mumbai, Santacruz (E), Mumbai 400098, India*
[3] *Homi Bhabha National Institute , Anushaktinagar, Mumbai 400094, India*
**Email: babajis@barc.gov.in*

We report an electron spin resonance (ESR) study in the MHz frequency domain on a single crystal of $Ca_3LiRuO_6$, recently proposed as a prototypical spin-orbit coupled oxide. In the antiferromagnetically ordered state with a noncollinear spin structure, which emerges below $T_N \approx 120$ K, we observe a ferromagnetic resonance (FMR) mode associated with the precession of weak ferromagnetic moments induced by spin canting. Upon rotating the magnetic field from parallel to the crystallographic *c*-axis to the perpendicular direction, the FMR mode shifts toward higher fields. This anisotropic behavior is consistent with antisymmetric exchange interactions of the Dzyaloshinskii-Moriya (DM) type, which are responsible for the spin canting.

**i0068**

**Study of Structural and Magnetic Properties of $Ca_{2-x}Pr_xMnTiO_6$ ($x$=0.0, 0.25, 0.5, 0.75, 1.0)**

Smita Borole*[1,2], Nilofar Kurawale[1,2], Rohan Kamble[1,2] and Sudhindra Rayaprol[1,2]

[1]*UGC-DAE Consortium for Scientific Research Mumbai Centre, BARC Campus, Mumbai 400085*
[2]*Savitribai Phule Pune University, Ganeshkhind, Pune - 411007*
**Corresponding Author Email: smita.borole1996@gmail.com*
The potential of double perovskites for practical applications particularly in thermoelectric and spintronic devices has encouraged intense research in recent years. In this study, the intricate correlation between structural and magnetic properties of the double perovskite oxides $Ca_{2-x}Pr_xMnTiO_6$ ($x$=0.0, 0.25, 0.50, 0.75, 1.0) has been studied. Single phase samples of title compounds $Ca_{2-x}Pr_xMnTiO_6$ ($x$=0.0, 0.25, 0.50, 0.75, 1.0) have been prepared by conventional solid-state reaction method. All the compounds crystallize into orthorhombic crystal structure, however the influence of increasing Pr content on the magnetic properties can be seen clearly. Overall, magnetization studies show that there is inherent magnetic frustration in the system and lack of long-range magnetic order, which is also supported by low temperature neutron diffraction studies. A comparison of the structural and physical properties of double perovskite compound is presented here to understand the strong correlation between structural and magnetic properties.

**i0069**
**X-Ray Diffraction And M-T Measurement of $Sr_3CuRu_2O_9$**
Himanshu Tanwar[1, a)], Sujata Sanghi1, [b)] and Ashish Agarwal1,[c)]
*1Department of Physics, Guru Jambheshwar University of Science and Technology*
*Hisar-125001, Haryana India*
*c) Corresponding author's email address – aagju@yahoo.com*
In this report we have synthesized a novel magnetic polycrystalline $Sr_3CuRu_2O_9$. Phase purity confirmed by X-ray diffraction and crystal structure studied with Rietveld refinement using Fullprof program, estimated space group *Pm-3m (221)* with cubic crystal structure. Copper/Ruthenium atoms were present in square geometry. In MT measurement hysteresis is expected on the basis of ZFC and FC curve, there is possibility of significant magnetic ordering below a temperature around 68K, thermodynamic irreversibility exists below 122K ($T_{irr}$). Difference between FC and ZFC increases with the lowering of temperature below $T_{irr}$.

**i0070**
**Interplay of Competing Magnetic Interactions in Modified $SrMnO_3$**
Rahul Kumar Sahu, Rohan Naitame and Dr. Oroosa Subohi [a)]
*Advanced Functional Materials Laboratory, Department of Physics, Visvesvaraya National Institute of Technology (VNIT), Nagpur,440010*
*[a)]Corresponding author: oroosa@phy.vnit.ac.in*
$SrMnO_3$ was synthesized by sol-gel auto-combustion method, and its compositional modifications were achieved by substituting Ba at the A-site and/or Fe at the B-site to obtain $Sr_{0.9}Ba_{0.1}MnO_3$, $SrMn_{0.9}Fe_{0.1}O_3$ and $Sr_{0.9}Ba_{0.1}Mn_{0.9}Fe_{0.1}O_3$ perovskites. Structural analysis confirmed the formation of phase-purity of $SrMnO_3$ with hexagonal symmetry (space group *$P6_3/mmc$*), while the co-doped composition exhibited indications of complex magnetic ordering. The observed two-step magnetization in $Sr_{0.9}Ba_{0.1}Mn_{0.9}Fe_{0.1}O_3$ is attributed to the coexistence of ferromagnetic and antiferromagnetic domains, likely driven by the mixed valence states of Mn ($Mn^{3+}/Mn^{4+}$) and Fe($Fe^{3+}/Fe^{4+}$) and the competition between superexchange and double-exchange interactions. Notably, the M-type magnetic hysteresis loop with dual coercive fields observed at room temperature is a rare phenomenon, suggesting the presence of magnetically decoupled regions or spin reorientation effects. Dielectric measurements revealed a maximum dielectric constant of 523 at 100 kHz for the co-doped sample, indicating magnetodielectric coupling.

**i0071**
**Aspects of Magnetism in Kagome Single Crystal $FeCr_3Te_6$**
M Lamba [a)], P Saha, K Yadav, S Patnaik [a)]
*School of Physical Sciences, Jawaharlal Nehru University, New Delhi-110067, India*
*[a)] Corresponding authors: manojl58_sps@jnu.ac.in, spatnaik@jnu.ac.in*
**Abstract.** $FeCr_3Te_6$ has gained attention due to its kagome ferromagnetic behavior driven by the structure and the interplay between topology and electronic correlations. Here we report the synthesis, structural, and magnetic properties of a single-crystalline ferromagnetic compound that is slightly off-stoichiometric compared to the parent $FeCr_3Te_6$. The space group is confirmed to be P-3m1. It has a Curie temperature of $T_c$ = 184 K that is higher than the previously reported one ($T_c$= 124 K), followed by an additional ferromagnetic transition near $T_{c2}$ = 52 K. We observe hysteresis behavior in magnetic field scans at a temperature of 2 K. With an increase in temperature, this hysteretic behavior is suppressed and completely vanishes at a temperature of 50K. In magnetization measurements, the compound also shows evidence of topological Hall effects, suggesting the presence of chiral spin texture or skyrmions in this centrosymmetric system.

**i0072**
**A Study of Angle Dependent Magnetization in Quasi-2D $EuRhAl_4Si_2$ Single Crystal**
Benjamin L. Fanai[1], Lalthansanga[1], J. Lalhlimpuia[1], Ruta Kulkarni[2], Arumugam Thamizhavel[2] and Arvind Maurya[1]
*[1]Department of Physics, School of Physical Sciences, Mizoram University, Aizawl 796 004, India*
*[2]Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai 400 005, India*

**Email: amaurya@mzu.edu.in*
We report angle dependent magnetization of the quaternary material $EuRhAl_4Si_2$ at temperature 2K with sample rotation in the *ac*-crystallographic plane with respect to the applied magnetic field. A high-resolution magnetization data measured in a vibration sample magnetometer reveals presence of miniature magnetization jumps observed in the one third magnetization plateau up to 45 degrees tilting off the c-axis towards the a-axis in the tetragonal crystallographic plane, while the hysteretic metamagnetic jumps corresponding to spin-flip leading to magnetic saturation persist well above 45 degrees. An inverse correlation between the plateau state magnetic susceptibility and appearance of miniature steps in magnetization is observed.

**i0073**

**Electronic and magnetic properties of kagome-type $DyMn_6Ge_6$ compound: an experimental investigation.**

Bashab Mukharjee[1] and Subham Majumdar[1, a)]
*[1]School of Physical Sciences, Indian Association for the Cultivation of Science, 2A and B Raja S. C. Mullick Road, Jadavpur, Kolkata 700 032, India.*
*[a)] Corresponding author: sspsm2@iacs.res.in*
We report on the magnetic and anisotropic magnetoresistance (AMR) properties of the layered kagome magnet $DyMn_6Ge_6$, a member of the $RMn_6Ge_6$ family with complex magnetic ordering. $DyMn_6Ge_6$ crystallizes in the hexagonal $HfMn_6Ge_6$-type structure (space group P6/mmm) and exhibits antiferromagnetic ordering with a Néel temperature of 450 K. At 293 K, it shows a ferrimagnetic spiral (FS) structure with antiparallel Dy and Mn layers, transitioning below 100 K to a triplet conical ferromagnetic spiral (FIM + FS) as moments tilt toward the c-axis. Strong magnetic anisotropy is observed, with distinct field-direction-dependent behaviors. ZFC and FC curves diverge sharply below ~100 K ($T_{FIM}$). The zero-field resistivity indicates metallic behavior, while large, non-saturating magnetoresistance (MR) is seen below 100 K positive for both direction ($H \perp c$ & $H \parallel c$) and negative above this temperature. Transport measurements reveal a pronounced AMR, highlighting a strong coupling between magnetic structure, spin-orbit interaction, and electronic transport, making $DyMn_6Ge_6$ a promising platform for spintronic studies.

**i0074**

**Spin-Polarized Flat Bands and Magnetic Moment Induction in Carbon-Doped Boron Monoxide Monolayer: A DFT Study**

Kuneh Shah[1, a)], Shreya G. Sarkar[2] and Brahmananda Chakraborty[3,4]
*[1]Department of Physics, Indian Institute of Technology, Roorkee 247667, Uttarakhand, India*
*[2]Accelerator & Pulsed Power Division, Bhabha Atomic Research Centre, Mumbai 400085, India*
*[3]Homi Bhabha National Institute, Mumbai 400094, India*
*[4]High Pressure and Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai, India-400008*
*[a)] Corresponding author: shah_kp@ph.iitr.ac.in*
Density Functional Theory (DFT) calculations were performed to investigate the effect of carbon doping on boron monoxide (BO) monolayers. Pristine BO, previously synthesized and reported in literature, exhibits an indirect bandgap of 2.24 eV, making it suitable for optoelectronic applications such as photodetectors. Our simulations reveal that carbon substitution at boron sites induces spin-selective conductivity, a tunable bandgap, and robust half-metallic behavior accompanied by a magnetic moment stable at room temperature. The study was designed with experimentally realistic formation energies and doping concentrations in mind. Comprehensive analysis using band structure, spin density distribution, and partial density of states elucidates the origin of these electronic and magnetic features, primarily linked to localized states introduced by the dopant. Notably, a ~22.6% reduction in work function was observed, indicating enhanced surface reactivity. If experimentally realized, carbon-doped BO could emerge as a promising platform for spintronic devices, magnetic data storage, and catalytic applications.

**i0075**

**Investigation on Magnetic and Transport Properties of CMT & CFT Huesler Alloy**

Chinmoy Biswas[1,a)], Avijit Tudu[1] , K. Suresh[2] ,B. Srinivas Rao3, A. Rajanikanth[1,*]
*1) School of Physics, University of Hyderabad, Gachibowli, Telengana, 500046*
*2) International Advanced Research Centre for Power Metallurgy and New Materials (ARCI), Hyderabad*
*3)NIT Warangal, Kazipet, Warangal, Telengana, 506004*
$X_2YZ$ Heusler alloys are one of the important class of alloys focusing major applications in spintronic. In this work we focused on the alloy $Co_2MnTi$ & $Co_2FeTi$, which also possess high Curie temperature and half metallic behaviour. We synthesized both of the alloy using arc melting technique. Then It had been quenched in cold water to achieve it's desired phase after annealing several times. Room Temperature XRD analysis confirms the presence of cubic crystal structure and EDS analysis confirms the uniformity of each components. The magnetization data indicates the soft ferromagnetic nature. The temperature fit to electrical resistivity data shows the absence of quadratic temperature dependence of resistivity, suggesting half metallic behaviour of CMT & CFT, making it one of a highly promising candidate for room temperature spintronic applications.

**i0076**

**Magneto-Transport And Mutual Inductance Studies In Boron-Doped Diamond Superconducting Film**

Sulagna Dutta
*Tata Institute of Fundamental Research, Mumbai (400005)*
**Email:sulagna.dutta@tifr.res.in*

We investigate the superconducting transport properties of boron-doped diamond films through a combination of current-voltage and magnetoresistance measurements. Clear signatures of a magnetic-field-induced superconductor–insulator transition (SIT) are observed, along with non-linear IV characteristics suggestive of a granular superconducting landscape. Additionally, two-coil mutual inductance measurements are used to extract the temperature dependence of the magnetic penetration depth $\lambda(T)$, providing insights into the superfluid stiffness and phase fluctuations near the transition.

**i0077**

**Low Temperature Glass–Like Arrestation Formed by Kinetic Arrest in Half Doped Manganites**

Himitri Trivedi[1], Bhargav Rajyaguru[2], Nisarg Raval[1], Uday Kareleeya[1], Apexa Maru[1], Mehul Parmar[1], Bharavi Hirpara[1], Keval Gadani[3], K. Asokan[4,5], A.D. Joshi[6], D.D. Pandya[7], Davit Dhruv[1], R.K. Trivedi[8], N.A. Shah[1], P.S. Solanki[1, *]

[1]*Department of Physics, Saurashtra University, Rajkot – 360005, India*

[2]*Devision of Solid State Physics, Department of Material Science and Engineering, Uppsala University, SE–751 03, Sweden*

[3]*Centre of Education, Indian Institute of Teacher Education (IITE), Gandhinagar–382016, India*

[4]*Department of Physics & Centre for Interdisciplinary Research, University of petroleum and Energy Studies (UPES), Dehradun, Uttarakhand 248007, India*

[5]*Inter University Accelerator Center, New Delhi, 110067, India*

[6]*Department of Nanoscience and Advanced Materials, Saurashtra University, Rajkot 360005, India*

[7]*UGC: Malaviya Mission Teacher Training Centre, Saurashtra University, Rajkot 360005, India*

[8]*Bahauddin Science College, Junagadh-362001, India*

** Corresponding author: piyush.physics@gmail.com*

The phase transition behavior of half–doped Nd0.5Sr0.5MnO3 (NSMO) manganite, exhibiting hysteretic temperature dependence of magnetization and resistivity at the nanoscale are yet to be studied. The NSMO sample was synthesized using the sol–gel method and sintered at ~ 1350 °C to achieve a nearly perfect crystalline structure. X–ray diffraction (XRD) analysis confirmed the orthorhombic crystal structure with space group Imma. Furthermore, X–ray absorption spectroscopy (XAS) provided insight into the local electronic and chemical environment around the Mn sites. A detailed magnetization study reveals a first–order phase transition from ferromagnetic metallic (FMM) to antiferromagnetic insulator (AFI) at low temperatures, with anomalies across the phase transition. The results indicate a glass–like arrest of kinetics at low temperatures, which significantly contributes to the thermomagnetic irreversibility observed in the system. A correlation between the hysteresis width and the applied magnetic field suggests a competition between kinetic arrest temperature and supercooling temperature. These findings offer new perspectives on the temperature–driven phase transitions in NSMO that enhances the understanding of magnetic behaviors of manganites.

**i0078**

**Field induced transition in CePdGe**

Priyanshi Tiwari[a)], Suman Karmakar, Vikas Nawari, Arvind Yogi and R. Rawat

*UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, India*

** priyanshitiwarima@gmail.com*

The analysis of powder X-ray diffraction data of polycrystalline sample CePdGe revealed TiNiSi-type orthorhombic structure. The PM state, at high temperature is characterized by large negative paramagnetic Curie temperature (-54.4 K) and effective paramagnetic moment of 2.32 $\mu_B$/f.u. In spite of clear signature of transition in magnetization, specific heat ($C_P$) shows a sharp peak at 3.2 K with a long tail at high temperature. With magnetic field, the peak position shifted to low temperature as expected for antiferromagnetic (AF) ordering. However, a hump around 5 K appears in the presence of magnetic field. It suggests suppression of AF order at the cost of ferromagnetically correlated regions. Consistent with this interpretation, a sign inversion of MR is observed at 3 K.

**i0079**

**Exploring The Effect Of Twist Angle In $Nb_{15}S_{30}$ Biflake Structure Via Ab-initio Calculations**

Samar Kapila[1, a)], Shiksha[1], Neha[1], Sheetal Dhiman[1], Anjali[1], Anjna Devi[2], Arun Kumar[1]

[1]*Govt. Degree College, Bilaspur, Himachal Pradesh, India, 174001*

[2] *Government degree college Baroh, Kangra HP, India, 176054*

**Email :05kapilsamar@gmail.com*

Twistronics explores how the relative twist between stacked layers influences the properties of low-dimensional materials. While this concept has been widely applied to infinite 2D systems, its effect on finite-sized flakes remains less studied. In this work, we investigate monolayer, bilayer, flake, and biflake forms of $NbS_2$ using first-principles calculations. Monolayer and bilayer structures show metallic and non-magnetic behaviour, whereas $Nb_{15}S_{30}$ flake and $Nb_{15}S_{30}$ biflake exhibits semiconducting feature. The magnetic moment of twisted $Nb_{15}S_{30}$ biflake increases when angle ranging from 1º to 15º which arises due to its edge-effect and $Nb_{15}S_{30}$ biflake get stabilized at an angle of 14º which suggests a possible magic angle. Hence, these results indicates the potential application of twisted biflakes for spintronic and nanoscale device applications.

**i0080**

**Penetration depth measurement of amorphous $Re_6Zr$ using coplanar waveguide technique**

Arghya Dutta[1,*,] and Pratap Raychaudhuri[1]

[1]*Tata Institute of Fundamental Research. Dr. Homi Bhabha Road, Navynagar,Colaba Mumbai Maharastra 400005 India*
** arghyaduttabku@gmail.com*
We present the study of the London penetration depth (λ) in a superconducting Re6Zr thin film using coplanar waveguide (CPW) resonance measurements and compare with the value obtained from two coil mutual inductance measurements. Both methods examine the electromagnetic response of the superconducting thin film but work at different frequencies and setups. Despite the differences in measurement approaches, the results are consistent within the superconducting state, confirming the reliability of the measurements. This validation offers a solid characterization of superconducting properties of an amorphous thin film.

**i0081**

**Ferrites : Perspectives from Terahertz Spectroscopy**

Parvathy J P[1,2], Sarang Joshi[1], Aryansingh Kushwah[1,2], Snehal Haldankar[1], Anol Mondal[1], Sudeep Tiwari[1*] and S.S.Prabhu[1]
*Department of Condensed Matter Physics and Material Science, Tata Institute of Fundamental Research, Mumbai,400005*
*[2]Department of Physics, IISER Berhampur, Ganjam, Odisha-760003*
**sudeep.tiwari@tifr.res.in, parvathy21@iiserbpr.ac.in*
This study investigates the magnetic and opto-dielectric properties of Zn0.5Fe2.5O4 nanoparticles (ZNF NPs) using Terahertz Time-Domain Spectroscopy (THz-TDS). Synthesized via the sol-gel method, ZNF NPs (~8 nm) exhibit a fcc cubic spinel structure, as confirmed by powder X-ray diffraction (PXRD). DC magnetization and M-H measurements reveal superparamagnetic behaviour at 300 K with a blocking temperature of ~154 K. THz-TDS analysis demonstrates a stable refractive index of 2.554 and a low extinction coefficient of 0.127, with real and imaginary dielectric constants of 6.5 and 0.67, respectively. The low loss tangent underscores ZNF NPs as promising candidates for terahertz-based electronic device applications. At DAE-SSPS 2025 conference, we will present expanded results, including discussions on other ferrites such as CoFe2O4, spanning hard to soft compositions and nanoscale to bulk forms.

**i0082**

**Magnetic properties and magnetocaloric effect in hexagonal compound of $NdNi_5$**

Anu [a)], Bhagyashree pol, and P. D. Babu
*UGC-DAE Consortium for Scientific Research, BARC, Mumbai 400085, India.*
*[a)]Email:anusheokand145@gmail.com*
Hexagonal intermetallic compound, $NdNi_5$, was prepared by arc melting technique and characterized by ac and dc magnetization, electrical transport measurements. Magnetization data reveals ferromagnetic order with transition temperature around 7.2 K. Magnetization does not saturate even in fields of 9T and magnetic moment at this field being much less than what is expected for Nd atom (as Ni atom in these compounds are not expected carry any moment). AC susceptibility data shows frequency dispersion indicative of magnetic glassy phase in the system below Tg ~ 5.9 K. Magnetocaloric effect calculated by using Isothermal magnetization exhibits a maximum of $-\Delta S_M^{pk}$ =8.5 J/kg-K for a field change of ΔH = 9 T. The universal scaling law predicted by mean field theory for second order phase transitions obey in this case. Metallic behavior was seen in electrical transport data and negative magnetoresistance was observed in the compound with a maximum value around $T_C$. Spin-disorder scattering is though to be mainly responsible for negative MR in this system.

**i0083**

**Observation of Magnetic Anomalies in vdW Antiferromagnet $MnPSe_3$**

Sreelakshmi M. Nair [1] and R. S. Patel [1, a]
*[1] Department of Physics, Birla Institute of Technology and Science, Pilani, K K Birla Goa Campus, Zuarinagar, Sancoale, Goa 403726, India*
*[a)] rsp@goa.bits-pilani.ac.in*
This work reports the structural and magnetic characterization of antiferromagnetic semiconductor $MnPSe_3$ crystals.
X-ray diffraction (XRD) was employed to investigate the structural properties of the material. Distinct magnetic anomalies and phase transitions are revealed through temperature and field-dependent magnetization measurements.

**i0084**

**Interplay of Charge Transport And Magnetism In $Pr_{0.5-x}Na_xSr_{0.5}MnO_3$ (x = 0, 0.5)**

Ramyashri and Mamatha D. Daivajna
*Department of Physics, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka, 576104, India.*
**Email:mamatha.daijna@manipal.edu*
The bulk polycrystalline $Pr_{0.5-x}Na_xSr_{0.5}MnO_3$ (x = 0, 0.05) samples were synthesized to study the effect of sodium substitution on the structural and transport properties. The samples shows tetragonal (I4/mcm) structure and minor secondary phase of $SrMnO_3$ at room temperature. The temperature-dependent electrical resistivity measured under a magnetic field of 0 and 90 kOe. The charge ordering observed in the $Pr_{0.5}Sr_{0.5}MnO_3$ sample is suppressed in the Na substituted sample. The first order nature of the ferromagnetic metallic to antiferromagnetic insulator transition is destroyed in $Pr_{0.45}Na_{0.05}Sr_{0.5}MnO_3$, which is evident from the absence of thermal hysteresis between the cooling and warming cycles.

**i0085**

**Evaluation of Structural and Magnetic Phase Transition in Ta Doped $Zr_{1-x}Ta_xFe_2$**

Vikas Singh[1*], Priyanshi Tiwari[1], Rajeev Joshi[1], R Rawat[1], A. K. Yogi[1]
[1]*UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, India*
**email nawarivikas@gmail.com*

We report the detailed structural, magnetic properties of Ta doped $Zr_{1-x}Ta_xFe_2$ ($x$ = 0.0, 0.2, 0.35, and 0.5) compounds by using of x-ray diffraction, dc-susceptibility, and magnetization. The polycrystalline ingots were prepared by the arc melting. The observed x-ray diffraction (XRD) patterns were fitted with cubic C-15 $MgCu_2$-type for Ta doping up to $x$ = 0.20 and hexagonal, C-14 $MgZn_2$ type Laves phase symmetry for Ta doping up to $x$ =0.35. However, the Ta doping at $x$ = 0.35 is found with mixed symmetry of cubic and hexagonal structure. Moreover, the unit-cell parameters were found to be decrease as we increase the doping concentration (x) is because of the difference in the ionic radii. Further, the magnetic properties show a clear phase transformation from ferromagnetic to antiferromagnetic transition for doping concentration $x$ = 0.5, most probably due to significant change might be accompanied by a drastic reduction of Fe-Fe bond lengths in $Zr_{1-x}Ta_xFe2$.

**i0086**

**Observation of Plateau-Like Magnetoresistance with Anomalous Hall Effect in Kagome Magnet $TbCo_2$**

P. Das, T. Kumari, M lamba, M. Yadav and Prof. S. Patnaik*
*School of Physical Sciences, Jawaharlal Nehru University, New Delhi-110067*
**Email:priya90939@gmail.com, spatnaik@jnu.ac.in*

Kagome lattice-based materials are being shown interest in the scientific community for their frustrated spin structure and the interesting emergent properties from it. The magnetic aspects of $TbCo_2$, which is a $RCo_2$ compound and has a Co Kagome lattice, were experimentally studied. $TbCo_2$ has a magnetic transition at 235 K which was confirmed with resistivity and magnetization measurements. Zero field resistivity, Magnetoresistance (MR) and Hall measurements were done. It showed highest negative magnetoresistance at $T = T_C$ (around 6%), while plateau-like MR was observed at low magnetic fields below $T_C$. Anomalous hall effect was observed which saturated around 1 T aligning with the Magnetization data. The MR of the compound was seen to be reduced dramatically as we went lower temperatures than the critical temperature 235 K. The reversal of the sign of MR at low temperatures (around 15K) can be related to the freezing of spins of Co atoms as seen in the magnetization.

**i0087**

***Synthesis of $MoS_2$ Flower-like Structure for Optoelectronic Application***

Ankita Dey[1,*] and R. Thangavel[1]
[1] *IIT ISM Dhanbad, Dhanbad, India*
**22dr0051@iitism.ac.in*

Two-dimensional transition metal dichalcogenides (TMDs), particularly $MoS_2$, meet these criteria through their semiconducting behavior, atomic-scale thickness, This thesis reports the hydrothermal synthesis and systematic characterization of $MoS_2$ nanostructures optimized for optoelectronic applications. 1:5 Mo:S molar ratio condition was studied at 190 °C. Structural and chemical analysis using XRD, XPS, Raman, FESEM, and UV–Vis spectroscopy revealed that the optimized 1:5 synthesis yielded phase-pure $MoS_2$ with improved crystallinity, minimal oxidation, and uniform nanoflower morphology. The results demonstrate the critical role of synthesis parameters in tailoring the structural and electronic quality of $MoS_2$. The optimized material offers a viable platform for future spintronic architectures and lays the foundation for doping, heterostructure engineering, and device integration.Bulk $MoS_2$ has a bandgap of ~1.2 eV and becomes a direct bandgap semiconductor (~1.8 eV) in monolayer form. This has created significant interest in using $MoS_2$ for optoelectronics and photodetectors.

**i0088**

**Defect-Driven Enhanced $d^0$ Ferromagnetism in Non-Magnetic Substituted p-Type $SnO_2$ Thin Films Under $O_2$-Rich Condition**

Shyamsundar Ghosh[1,*]
[1]*Department of Physics, Bejoy Narayan Mahavidyalaya, The University of Burdwan, P.O.-Itachuna, Hooghly-712147, India*
**sghoshphysics@gmail.com*

Influence of non-magnetic cationic substitution under $O_2$-rich atmosphere on the structural defects and correlated $d^0$ ferromagnetism (FM) in p-type $Sn_{1-x}In_xO_2$ ($x \leq 0.1$) thin films fabricated by pulsed laser deposition are investigated. Beyond x > 0.02, $Sn_{1-x}In_xO_2$ film switches from n-type to p-type conductivity and simultaneously exhibited enhanced FM with magnetic moment as large as 15.21 emu/cm$^3$ and $T_C$ around 538 K for x = 0.08. Various spectroscopic techniques had detected the formation of Sn vacancy ($V_{Sn}$) defects as the consequence of In-substitution ($In_{Sn}$) under $O_2$-rich atmosphere. Magnetic spin-spin RKKY-type ferromagnetic interaction between the near-by $V_{Sn}$ or $V_{Sn}$ associated defect complexes be mediated through the localized holes due to $In_{Sn}$ defects. Beyond x > 0.08, stabilization of donor-type $In_i$ and $Sn_i$ defects had reduced the effective hole concentration and consequently the FM signal. Therefore, such high-$T_C$ enhanced FM in $SnO_2$-based oxide semiconductors can open up new opportunities in the field of dilute magnetic semiconductors and spintronics in future.

**i0089**

**Phase Evolution and Magnetic Frustration in Tunnel-Structured $Ba_{1.3}Mn_8O_{16}$**

Vishesh Sharma1, a), Gaurav Gautam1, Ahmad Raza2 and Shivani Sharma2
[1]*Department of Physics, Graphic Era Hill University, Dehradun 248002, India.*
[2]*National High Magnetic Field Laboratory, Tallahassee, FL 32310, United States.*
*a)Corresponding author: phy.vishesh@gmail.com*
Synthesis, crystal structure and magnetic behaviour of $Ba_{1.3}Mn_8O_{16}$ (BMO) is presented here. BMO crystallizes in monoclinic structure at room temperature, confirmed via X-ray diffraction and scanning electron microscopy (SEM) equipped with energy dispersive analysis of X-ray (EDX). Small, rod-shaped single crystals were crushed to confirm the crystal structure at room temperature using powder X-ray diffraction. Magnetic susceptibility measurements performed on the bulk sample reveal antiferromagnetic (AFM) ordering of Mn ions at low temperatures, indicating the presence of long-range magnetic interactions in the system.

**i0090**

**Crystal Electric Field Analysis of $CeRu_2Ge_2$**

Shovan Dan[1,a)], Gourav Dwari[1], Suman Nandi[1], Ruta Kulkarni[1], P.D Babu[2], A. Thamizhavel[1,b)]
[1]*Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai 400005, India*
[2]*UGC DAE Consortium for Scientific Research Mumbai Centre, 246 C,Common Facility Building BARC Campus, Mumbai 400085, India*
*Corresponding authors: [a)]dan.shovan@gmail.com, [b)] thamizh@tifr.res.in*
We report a detailed anisotropic studies on the magnetic properties of $CeRu_2Ge_2$ single crystal grown by the Czochralski method. At low magnetic fields, in addition to the known ferromagnetic transition at $T_C$ = 7.5 K, an additional antiferromagnetic (AFM) anomaly emerges at $T_N$ = 8.1 K. This AFM ordering is highly fragile, being suppressed under higher magnetic fields, and is absent in the specific heat data. The pronounced anisotropy observed in the magnetic susceptibility and magnetization along the [100] and [001] directions is quantitatively explained within the crystal electric field (CEF) framework using the point-charge model. The analysis reveals a CEF level scheme comprising three doublets, with a ground state and excited states at 458 and 593 K.

**i0091**

**Tuning the Lattice to Harness Magnetism: Structural–Magnetic Interplay in $A_2CoMnO_6$ (A = Ho, Lu)**

*R. Athira[1,2*], [1] S. D. Kaushik[1]
[1]*UGC-DAE Consortium for Scientific Research, Mumbai Centre, 246 C Common Facility Building, BARC, Mumbai India 400085.*
[2]*Savitribhai Phule Pune University Ganeshkhind, Pune -411007, Maharashtra, India.*
* athiraraghu92@gmail.com , sdkaushik@csr.res.in
Double perovskite compounds have shown intriguing physical properties owing to numerous possibilities of placing ions at various sites. Here double perovskites $Ho_2CoMnO_6$ and $Lu_2CoMnO_6$ compounds have shown structure induced modification in magnetic properties, which lead to alter physical properties significantly. We intend to focus on identifying the microscopic origin of the phenomenon through magnetic structure studies. The title compounds were synthesized by solid state reaction method. The phase purity of synthesized sample has been studied by x-ray diffraction and neutron diffraction under ambient conditions and it was found to be crystallized in monoclinic crystal structure with space group $\boldsymbol{P2_1/n}$ **(sg#14).** The temperature and magnetic field dependent magnetization were studied by employing the vibrating sample magnetometer (VSM) attached with commercial physical property measurement system (PPMS) to ascertain magnetic properties, which indicates magnetic transition ~30 K for $Lu_2CoMnO_6$ and ~80 K for $Ho_2CoMnO_6$. The temperature dependent neutron diffraction and other physical characterizations like magneto-dielectric study are being studied to understand multifunctional behavior in title compound**.**

**i0092**

**Synchrotron-based X-Ray Spectroscopy Characterizations of $Co_{35}Cr_5Fe_{10}Ni_{30}Al_{20}$ Magnetic High Entropy Alloy**

Rohit R. Shahi, Priyanka Kumari
*Functional and Energy Materials Research Laboratory, Department of Physics, Central University of South Bihar, Gaya, India*
It is now well known that the magnetic properties of High Entropy Alloys (HEAs) are significantly affected by the annealing. $Co_{35}Cr_5Fe_{10}Ni_{30}Al_{20}$ HEA was synthesized through the mechanical alloying technique and the synthesized HEA, exhibited mixture of fcc and bcc phase. The value of $M_s$ and $H_c$ for the synthesized HEA was found to be 42 emu/g and 18 Oe respectively. However, for $Co_{35}Cr_5Fe_{10}Ni_{30}Al_{20}$ HEA annealed at 700°C, the volume phase fraction of bcc phase increased and the fcc phase decreased. Along with the increase in bcc phase the value of Ms increased by more than 100 %. We investigated element specific magnetization through X ray magnetic circular dichroism (XMCD) for the as synthesized and annealed sample. We found that after annealing the magnetic moment corresponding to Fe and Ni enhanced significantly. The detail reason behind the change in magnetic properties of $Co_{35}Cr_5Fe_{10}Ni_{30}Al_{20}$ HEA after annealing and element specific magnetization is discussed in this study.
Keywords: High Entropy Alloys, Magnetic Properties, X-Ray Magnetic Circular Dichroism, Valence Band Spectra, Annealing.

**i0093**

**Effect of Mn addition on Magnetic and Corrosion Properties of $Co_{35}Cr_5Fe_{10}Ni_{30}Ti_5Al_{15}$ High Entropy Alloy**

Priyanka Kumari, Rohit R Shahi*

*Functional and Energy Materials Research lab, Department of Physics, Central University of South Bihar Gaya*
High Entropy Alloys (HEAs) consists of five or more than five principal elements in nearly equi-atomic ratio having concentration in the range of 5 to 35 at% [1] . However, conventional alloys have one or two principal elements and the properties of conventional alloys, governed by one major element along with some minor elements [1]. Thus, for conventional alloys there is less room to tune the multifunctional properties. On the other hands HEAs possessed multiple principal elements and hence provide great freedom to tune the multifunctional properties [1]. Extra ordinary properties of HEAs are mainly governed by the four core effects: high entropy effect, sluggish diffusion, severe lattice distortion and the cocktail effect. We systematically investigated the magnetic properties of FeCoNiTi based HEAs and optimized $Co_{35}Cr_5Fe_{10}Ni_{30}Ti_5Al_{15}$ HEA by the addition of alloying element, variation of composition of the alloying element and by annealing at different temperature for different duration [2]. The value of Ms was found 75 emu/g and Hc=18 Oe for as-synthesized $Co_{35}Cr_5Fe_{10}Ni_{30}Ti_5Al_{15}$ HEA [2]. However, for 700 °C annealed $Co_{35}Cr_5Fe_{10}Ni_{30}Ti_5Al_{15}$ HEA the value of Ms and Hc was increased to 94 emu/g and 41Oe respectively [2]. In this study we further extended our study and investigated the effect of addition of different amount of Mn (7.5) for Al (7.5) in $Co_{35}Cr_5Fe_{10}Ni_{30}Ti_5Al_{15}$ HEAs on phase formation, and magnetic properties [3]. XRD analysis confirmed the formation of fcc phase with minor concentration of σ phase for $Co_{35}Cr_5Fe_{10}Ni_{30}Ti_5Al_{7.5}Mn_{7.5}$ HEA. The value of saturation magnetization and coercivity is 83 emu/g & 6 Oe for $Co_{35}Cr_5Fe_{10}Ni_{30}Ti_5Al_{7.5}Mn_{7.5}$ HEA and the value of Ms significantly increased to 109 emu/g for 700 °C annealed $Co_{35}Cr_5Fe_{10}Ni_{30}Ti_5Al_{7.5}Mn_{7.5}$ HEA. However, no significant change was observed in the value of Hc after annealing. The synthesized $Co_{35}Cr_5Fe_{10}Ni_{30}Ti_5Al_{7.5}Mn_{7.5}$ HEA exhibits good corrosion resistance in 1 M NaCl, with a corrosion rate of 0.028 mm/y [3].

**i0094**

**Investigation of Structural, Transport and Magnetic Properties of Pyrochlore Iridates $Gd_2Ir_2O_7$**

H. Pradhan[1], R.K. Patel[1], A.G.A. Rahman[1], S. Behera[1], A.K. Pramanik[1]
[1]*School of Physical Sciences, Jawaharlal Nehru University, New Delhi-110067, India*
**Email:haraprasadpradhan25@gmail.com*

We have investigated the structural, electrical transport, and magnetic properties of pyrochlore iridates. Structural characterization of $Gd_2Ir_2O_7$ was carried out using X-ray powder diffraction followed by Rietveld refinement, confirming a cubic crystal structure with space group $Fd\bar{3}m$. In this compound, $Gd^{3+}$ ions possess seven 4f electrons, while $Ir^{4+}$ ions contain five 5d electrons. Electrical transport measurements, performed using the four-probe method, reveal a semimetal-like insulating behaviour. Magnetic measurements indicate an antiferromagnetic ordering with a transition temperature near 127 K. The intrinsic geometrical frustration of the pyrochlore lattice, combined with strong spin–orbit coupling from Ir atoms, plays a dominant role in determining the magnetic behaviour. The insulating nature is supported by resistivity analysis, while the paramagnetic response above the transition temperature is confirmed through magnetization and inverse susceptibility studies.

**i0097**

**Magnetic and Optical Properties of Rare-earth Dichalcogenide Compound, $CeSe_2$**

Smita Gohil, K. K Iyer, Shankar Ghosh, Kalobaran Maiti
*Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Dr. Homi Bhabha Road, Colaba, Mumbai-400005*
**Email: smitagohil@tifr.res.in, kbmaiti@tifr.res.in*

We present the magnetic and optical properties of single-crystalline $CeSe_2$, a rare-earth dichalcogenide crystallizing in a $ZrCuSi_2$-type tetragonal structure (space group P4/nmm). The compound exhibits antiferromagnetic ordering near 6 K, accompanied by magneto-crystalline anisotropy revealed by the measurements along two crystallographic directions. Magnetization measurements indicate the presence of a field-induced, disorder-broadened exceptional magnetic transition; understanding of this scenario requires detailed further study. Raman spectroscopy measurements show signature of possible spin phonon coupling and needs to be investigated further indicating it to be a candidate material for spintronic applications.

# j) Energy and environmental materials

**j0001**

**Growth and Structural Characterization of CZTS Crystal by Three-Zone Vertical Bridgman Technique**

Jay Sharma[1,2] and Satyaban Bhunia[1,2]

[1]*Surface Physics and Material Science Division, Saha Institute of Nuclear Physics, 1/AF, Bidhannagar, Kolkata 700064 India*

[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094 India*

[*] *Email: satyaban.bhunia@saha.ac.in*

Stoichiometric $Cu_2ZnSnS_4$ (CZTS) crystals were successfully synthesized using a three-zone vertical Bridgman furnace. The crystals exhibited a conical morphology with a well-formed crystallization front. X-ray diffraction (XRD) analysis confirmed the kesterite CZTS phase, with strong reflections from the (112), (220), and (312) planes and no detectable secondary phases. Raman spectroscopy revealed characteristic $A_1$ vibrational modes at ~288 $cm^{-1}$ and ~338 $cm^{-1}$, confirming the single-phase kesterite structure. The optimized thermal gradient in the furnace minimized compositional inhomogeneity and improved the crystal quality. These results demonstrate that the vertical Bridgman method can effectively produce high-quality CZTS crystals for photovoltaic applications.

**j0003**

**Boosting Oer Kinetics Through Cobalt Doping In $SrMnO_3$ Perovskite Oxides**

Poonam Moar [A], Bhimaraya R Biradar[b], Partha Pratim Das[b], Sourabh Barua[a,*]

[a] *Department of Physics, Central University of Punjab, Bathinda 151401, India.*

[b] *Low Dimensional Physics Laboratory, Department of Physics, National Institute of Technology Karnataka, Surathkal 575025, India.*

**Corresponding author: Sourabh.barua@cup.edu.in*

The oxygen evolution reaction (OER) plays a significant role in water splitting, and addressing its sluggish kinetics necessitates the development of highly efficient and stable electrocatalysts. Perovskite oxides have gained significant attention as cost-effective alternatives to noble-metal catalysts due to their tunable electronic structures and abundant active sites. In this study, cobalt-doped $SrMn_{1-x}Co_xO_3$ (x = 0,0.25,0.50,0.75,1) was synthesized via a sol–gel method to enhance its OER activity. Co substitution at the Mn site introduces mixed-valence states ($Mn^{3+}/Mn^{4+}$ and $Co^{2+}/Co^{3+}$), improving electronic conductivity and facilitating faster charge transfer. X-ray diffraction confirmed the retention of the perovskite structure, while FE-SEM and EDX show the morphology and elemental composition of the sample. Electrochemical measurements in 1 M KOH demonstrated that 50 % Co-substituted exhibited the lowest overpotential of 337 mV at 10 mA $cm^{-2}$, smallest Tafel slope of 101 mV/dec, and an electrochemical active surface area (ECSA) of 24.6 $cm^2$. This work demonstrates that 50 % Co doping is an effective strategy to boost the intrinsic OER activity as compared to pristine $SrMnO_3$, making it a promising non-noble-metal electrocatalyst for OER.

**j0004**

**Magnetocaloric Properties of Colossal Magnetoresistive Manganites ($Re_{1-x}A_xMnO_3$): A Variational Treatment**

Sunil Panwar [1,a)] and Rahul Saini[2]

[1, 2]*Department of Applied Science, Faculty of Engineering & Technology, Gurukula Kangri (Deemed to be University), Haridwar-249404, India*

[a)]*Corresponding author:dr.sunilpanwar66@gmail.com*

By using Variational method, we have studied the role of magnetic field on magnetic entropy change ( $-\Delta S_M$) 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. From our results, we find that the magnetic entropy change *(-* $\Delta S_M$) increases with increasing temperature for a particular value of magnetic field *'h' & 'm'* parameters showing the sharp peak at low temperature & finally decreases at higher temperatures. The sharpness of the peak increases with increasing the '*h' & 'm'* values. In the present study, - $\Delta S_M$ reaches a peak value of about 1.4 J/ Kg K at a temperature $T_c \sim 200$ K for magnetic field parameters '*h'*=0.05 & '*m'*=0.5 with doping $x$=0.3, $V=0.1$ & $J_H=1.0$. It is seen that our results are in good agreement qualitatively with the experimental results. The double exchange interaction & spin-lattice coupling are the main mechanisms that control the magnetic & transport properties of these magnetic materials.

Keywords: CMR Manganites; Anderson Lattice Model; Magnetic Entropy Change; Variational Method; Magnetocaloric Properties

**j0005**

**Gamma Radiation Induced Synthesis of Cu and Ag Decorated Polyaniline for Thermoelectric Applications**

Sajid Ahmad*

*Nuclear Research Laboratory, Astrophysical Sciences Division, Bhabha Atomic Research Centre, Zakura, Srinagar, Jammu and Kashmir, 190024, India*

**Email:sajid@barc.gov.in*

In this study, we have successfully synthesized gamma radiation induced polyaniline (PANI) and copper/silver-decorated polyaniline samples. The single-pot in-situ synthesis approach allows the polymer and its composite to be synthesized in a pure form, without the need for any initiators or complex procedures. Gamma irradiation of the solution mixture produces both oxidizing and reducing species. In this environment, the Cu and Ag ions and aniline undergoes reaction simultaneously in a single pot,

resulting in the formation of Cu/Ag-decorated PANI. The oxidizing species initiate the in-situ polymerization of aniline without the need for an external oxidizing agent, while the reducing species convert metal ions into neutral metal atoms, which become incorporated into the polymer matrix. The resulting samples were subjected to structural characterization using X-ray diffraction and thermoelectric property measurements. The Cu/Ag-decorated polyaniline sample exhibited the highest power factor of ~ 4.48 $\times 10^{-2}$ μW/m·K² at 300 K, which is nearly 13 times higher than that of pristine polyaniline.

**j0006**

**First Principle Study of Hydrogen Storage in Lithium-decorated [4]cycloparaphenylene**

Smruti Ranjan Parida[1], and Sridhar Sahu[1], *

[1]*Computational Materials Research Lab, Department of Physics, Indian Institute of Technology (ISM) Dhanbad, Jharkhand-826004, India.*

**Email:sridharsahu@iitism.ac.in*

In this work, we use dispersion-corrected density functional theory calculations (DFT + D3) to examine the hydrogen storage performance of Li-decorated [4]cycloparaphenylene ([4]CPP). With a binding energy of 2.98 eV, two Li atoms are decorated over [4]CPP, and up to five $H_2$ molecules can be stored by each Li atom at an average adsorption energy of 0.17 to 0.07 eV/$H_2$. It is determined that the system's maximum hydrogen gravimetric capacity is 6.08 wt%. According to simulations using Atom-Centred Density Matrix Propagation molecular dynamics (ADMP-MD), at 300 K, the $H_2$ molecules desorb from [4]CPP. Adsorption results in a negligible change in the structure of [4]CPP+2Li, which ensures the system's stability.

**j0007**

**Density Functional Theory Insights into the Photocatalytic Activity of $C_2N$ Monolayer under $O_2$ and $O_3$ Exposure**

Soumendra Kumar Das[1*], Lokanath Patra[2], Prasanjit Samal[3] and Sridhar Sahu[1]

[1]*Department of Physics, Indian Institute of Technology (Indian School of Mines) Dhanbad, India*

[2]*G. W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA 30332, USA*

[3]*School of Physical Sciences, National Institute of Science Education and Research (NISER), Bhubaneswar, HBNI, Jatni, Khurda-752050, Odisha, India*

**Email: soumendra1591@gmail.com*

This article focuses on the photocatalytic water splitting activity of $O_2$ and $O_3$ adsorbed $C_2N$ monolayer using DFT. The band edge positions for both systems satisfy the condition for water splitting by spanning the water redox potential value. The optical absorption spectra indicate a blue shift with respect to the pristine sample and lie in the visible region. The calculated HSE-06 band structure exhibits a larger band gap for the dissociated structure, indicating a strong hybridization of the C-O bond. The present work sheds light on the use of oxidized/ ozonized $C_2N$ monolayer for its potential applications in water splitting for hydrogen production.

**j0008**

**Metal Decorated $TiO_2$ Nanotubes For Enhanced Solar-Driven Photoelectrochemical Water Splitting**

Bheem Singh,[1,2] Pooja Rani, [1,2] Somnath C. Roy,[3] Sunil Singh Kushvaha[1,2] a)

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

[2]*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, India 201002.*

[3] *Semiconducting Oxide Materials, Nanostructures and Tailored Heterojunctions (SOMNaTH) Lab, Department of Physics, Indian Institute of Technology Madras, Chennai, India 600036.*

*a) Corresponding author E-mail: kushvahas.nplindia@csir.res.in*

Photoelectrochemical (PEC) water splitting holds great promise for sustainable hydrogen production, yet the efficiency of conventional photoanodes remains limited by poor visible light absorption and rapid charge carrier recombination. In this work, we present metal-decorated $TiO_2$ nanotubes (TNTs) as efficient photoanodes for enhanced solar-driven PEC water splitting. TNTs were fabricated and subsequently decorated with metallic Pt and Zn films to improve charge separation and catalytic activity. Comprehensive structural and surface analyses confirm the successful decoration of the TNT surface with uniformly dispersed metal particles. Under solar illumination, Pt-decorated TNTs exhibits a photocurrent density of 135 μA/cm$^2$, while Zn-decorated TNTs achieves 118 μA/cm², both showing an improvement compared to bare TNTs (70 μA/cm$^2$). The enhanced performance is attributed to efficient interfacial charge transfer, and suppressed recombination due to the formation of metal-semiconductor Schottky junctions. These results demonstrate the potential of metal decoration as a straightforward and effective strategy to boost the PEC efficiency of $TiO_2$-based photoanodes for solar hydrogen production.

**j0009**

**Innovative Reverse Electroplating for Recycling Diamond-Coated Wire: Diamond Removal and Stainless Steel Recovery**

Bharathwaj Murugesan, Karuppasamy Pichan *

*Department of Physics, SSN Research Centre, Sri Sivasubramaniya Nadar College of Engineering, Chennai-603110, India.*

** E-mail: karuppasamyp@ssn.edu.in*

Diamond coated wire (DCW) has been widely used in various industries such as semiconductors, photovoltaics and ceramics for cutting and slicing. Notably, the increasing demand for these wires has led to a significant amount of waste generation. The disposal of used DCW raises significant environmental concerns, including waste accumulation through landfilling, potential toxicity, and

resource depletion. Furthermore, the economic implications are substantial, resulting in the loss of valuable materials and increased production costs. In this study, we present a new method for recovering waste DCW by extracting diamond particles and stainless steel (SS) wire by removing the Ni coating using the reverse electroplating (REP) process. In this technique, process parameters such as acid concentration (mole), time (minutes), temperature (°C), and current density (A dm−2) are optimised to achieve better efficiency. The surface morphology of the DCW was investigated using X-ray diffraction (XRD), Raman spectroscopy, optical microscopy and scanning electron microscopy (SEM). The metal layers and their composition were investigated using energy dispersive X-ray spectroscopy (EDX) and X-ray photoelectron spectroscopy (XPS) analyses. After the REP, the particle size distribution of the retrieved diamond particles and the thickness of the SS wire core were measured. The removal efficiency for the nickel coating and diamond particles from the wire was calculated.

**j0010**

**Gold-Iron Bimetallic Electrocatalysts Assembled on MWCNT for Borohydride Oxidation Reaction in Fuel Cell**

Bilwadal Dutta[1, 2], Chandan Kumar Raul[1], and Ajit Kumar Meikap[1]
[1]*Department of Physics, National Institute of Technology, Durgapur, West Bengal, India*
[2]*Department of Physics, Michael Madhusudan Memorial College, Durgapur-713216, West Bengal, India*
**Email: akmeikap.phy@nitdgp.ac.in*

Herein, we report the electrochemical performance of Au/MWCNT and AuFe/MWCNT electrocatalysts for the borohydride oxidation reaction in fuel cell applications. The bimetallic electrocatalysts show superior current density 23.58 mA $cm^{-2}$, higher electrochemically active surface area (ECSA) 2502.83 $cm^2$ $mg^{-1}$, mass activity (MA) 2358.23 mA $mg^{-1}$, and surface activity (SA) 0.009 mA $cm^{-2}$ over the monometallic electrocatalysts. EIS spectra also reveal that AuFe/MWCNT have a lower charge transfer resistance ($R_{ct}$) 61.50 ohm value compared to Au/MWCNT. The evaluated electrochemical parameters suggest that AuFe/MWCNT is a valuable and more cost-effective electrocatalyst for direct borohydride fuel cells (DBFCs) applications.

**j0012**

**$LiFePO_4$ thin film as anode of Li ion Batteries**

C. Nayak[1,2,a)], S. Atwal[1,2], A. Biswas[1,2], R. B. Tokas[1,2] and D. Bhattacharyya[1,2]
[1]*Atomic and Molecular Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, India.*
[2]*Homi Bhabha National Institute, Anushakti Nagar, Mumbai 400094, India*
[a)]*Corresponding author: nayakc@barc.gov.in*

$LiFePO_4$ (LFP) thin films were deposited on Pt coated SS substrates by RF Magnetron Sputtering. The thickness and structure of the films were determined by UV-Vis spectrophotometry and GIXRD measurements respectively. Solid state thin film electrolyte $Li_3PO_4N$ (LIPON) was deposited on LFP/Pt/SS by RF reactive magnetron sputtering using $Li_3PO_4$ target under nitrogen atmosphere. Lithium-ion half cells were prepared using both the LFP thin film and LFP/LIPON bi-layer and battery performance were tested by galvanostatic charge-discharge (GCD) measurements. Electrochemical Impedance spectroscopy (EIS) was done to evaluate the impedance characteristics of the films.

**j0013**

**Up-Conversion Behavior Of $Nay(Yb,Er)F_4$ In Presence Of $Tho_2$ Matrix**

Sourav Majumder[1,2], Dheeraj Jain[1] and V. Sudarsan[1,2,*]
[1]*Radiation & Photochemistry Division, Bhabha Atomic Research Centre, Mumbai-400 085.*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai-400 094.*
**vsudar@barc.gov.in*

Optical properties of rare-earth doped sodium yttrium fluoride up-converting material (UCM), have been investigated in presence of thorium dioxide. Mechanically milled samples comprising nuclear-grade $ThO_2$ powder and $Yb^{3+}$, $Er^{3+}$ co-doped bulk $NaYF_4$ were prepared wherein UCM fraction (wt.%) was varied over 1 to 100. Irradiation of as-milled mixtures as well as UCM by 980 nm laser showed characteristic up-conversion emissions in visible region (520 nm, 540 nm, 655 nm). Ratio of Red (655 nm) to Green (520 nm & 540 nm combined) emission (R/G) increased with UCM fraction. In stark contrast to UCM or UCM-rich mixtures, Power (laser) dependent measurements on UCM-lean mixtures showed saturation in R/G. Results also showed that average number of NIR photons involved for both, green and red emission increase with (a) temperature and (b) increasing UCM fraction. The effect has been explained in terms of local temperature rise in UCM particles and heat transport through surrounding $ThO_2$ matrix.

**j0014**

**Lithium Ion Diffusion and Anharmonic Phonons in α-$Li_3N$**

Chanchal,[1,2,*] Mayanak K.Gupta,[1,2] Ranjan Mittal,[1,2] Samrath L. Chaplot[1,2]
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400085, India*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*
**chanchaltomer66@gmail.com*

α-$Li_3N$ is a promising Li ion superionic conductor for battery applications due to its high ionic conductivity. This study investigates the role of different Li Wyckoff sites in influencing the ionic transport using machine learned molecular dynamics simulation. We found that below 600 K, the Li at 2*c* Wyckoff site contribute dominantly to diffusion in ab-plane. However, at elevated temperature

Li at both the sites (2*c* and 1*b*) becomes equally mobile and in turn leading to 3-D superionic behaviour. We identified that the superionic transition accompanied by the breakdown of a few key phonon modes.

**j0015**

**Defect Engineering and Photoluminescence Enhancement in $Eu^{3+}$-Doped $Ca_2GeO_4$ via Alkali Ion Co-doping**

Bhavana Bharti[1,2,a] , Ananya Naik[3], Mohit Tyagi,[2,4] Santosh K. Gupta,[1,2] and K. Sudarshan[1,2,b]
[1]*Radiochemistry Division, Bhabha Atomic Research Centre, Trombay, Mumbai – 400085, India*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai – 400094, India*
[3] *Institute of Chemical Technology, Matunga Mumbai 400019, India*
[4]*Technical Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai – 400085, India*
[a]*bhavanab@barc.gov.in*; [b]*kathis@barc.gov.in*

In this study, we investigate the effect of K+ co-doping on the structural and luminescent properties of $Eu^{3+}$-doped Ca2GeO4. X-ray diffraction confirmed the formation of phase pure samples, while FTIR spectra revealed the presence of $CaO_6$ distorted octahedra and GeO4tetrahedra, characteristic of the host lattice. The emission spectra exhibited the characteristic transitions of $Eu^3$, with the electric dipole transition $^5D_0 \rightarrow {}^7F_2$ dominating, indicating that $Eu^{3+}$ions occupy sites lacking inversion symmetry. The material exhibits both photoluminescence and radioluminescence, and the overall PL emission intensity is significantly enhanced by $K^+$ co-doping due to charge compensation via partial substitution of $Ca^{2+}$ ions.

**j0017**

**Role of soft phonons in Li-ion diffusion: Crystalline and amorphous $LiAlSiO_4$**

M K Gupta[1,2], S Kumar[1,2], C Tomar[1,2], S Malgope[1,2], R Mittal[1,2], S L Chaplot[1,2]
[1] *Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India*
[2] *Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*
*Email:mayankg@barc.gov.in*

This study investigates lithium-ion diffusion in both crystalline and amorphous phases of $LiAlSiO_4$, with a particular focus on the influence of host lattice dynamics. Using machine-learned molecular dynamics (MLMD) and ab initio molecular dynamics (AIMD) simulations, we analyze the atomic-scale mechanisms governing Li-ion transport. Our results reveal that the crystalline phase exhibits non-diffusive behavior below 600 K and transitions to superionic conductivity above this temperature. In contrast, the amorphous phase demonstrates significant Li-ion diffusion even at lower temperatures. Constrained dynamics simulations show that oxygen atom vibrations play a critical role in facilitating Li-ion mobility, highlighting the importance of soft phonons in enhancing ionic conductivity. These findings underscore the potential of amorphous $LiAlSiO_4$ as a promising solid electrolyte for next-generation solid-state batteries.

**j0018**

**Anisotropic one-dimensional curved diffusion in $Li_{1-x}FePO_4$ (x = 0.25,0.4): a machine-learned molecular dynamics study.**

Prabhatasree Goel[a)], M K Gupta, R Mittal and S L Chaplot
*Solid State Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400085, India*
[a)]*Corresponding author: knp@barc.gov.in*

Lithium transition metal phosphor-olivines are useful electrode materials, owing to their stability, high safety, low cost and cyclability. Here we report studies of the diffusion behavior of fully lithiated and delithiated olivines compounded using large-scale machine learned molecular dynamics simulations. We have used these studies to understand the effect of delithiation on diffusivity of Li atoms, which are crucial in their applications as cathode materials. Both our experimental and theoretical simulations conclude that the olivines are stable even after about 60% delithiation. Stochiometric $LiFePO_4$ does not show any macroscopic diffusion even at high temperatures of 700 K. But as lithium is delithiated from the olivine structure, we find that Li diffusion increases and macroscopic diffusion occurs at around 700 K with increasing delithiation. Using machine learned molecular dynamics studies we have visualized the curved 1-Dimensional pathway of Li migration. This corroborates the experimental observations of neutron diffraction by Nishimura[1] et al. Our studies conclusively indicate anisotropic diffusion in delithiated LiFePO4. This study also infers that the olivine structure is stable and impervious to local disorder in the fully stoichiometric analogue even with increasing temperature.

**j0019**

**Mechanistic Insights into Lithium Intercalation Pathways in rGO-$MoS_2$ Composite Through Operando X-Ray Investigations**

Ashok Kumar Yadav[1,2, a)], A. K. Tyagi[3], V. Shrihari[4] and D. Bhattacharyya[1,2]
[1]*Atomic and Molecular Physics Division, Bhabha Atomic research Centre, Mumbai - 400084, India*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai-400094, India*
[3] *Chemistry Division, Bhabha Atomic Research Centre, Mumbai 40008.*
[4]*High Pressure & Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Mumbai, 400085, India*
**Email:akyadav@barc.gov.in*

A $MoS_2$-reduced graphene oxide (rGO) composite was synthesized using a single-source molecular precursor to enhance the electrochemical performance of $MoS_2$-based anodes for lithium-ion batteries (LIBs). Electrochemical tests of the LIB prepared

with $MoS_2$@rGO showed high initial discharge capacity (668.85 mAh/g) and excellent cycling stability with >99% Coulombic efficiency after the third cycle. *Operando* Mo K-edge X-ray absorption spectroscopy measurements during the discharge/charge cycle of the LIB confirmed a reversible redox transition between $Mo^{4+}$ and $Mo^0$, highlighting a two-step lithiation/de-lithiation process while *operando* X-ray diffraction measurement revealed the formation of an intermediate phase also. The rGO framework plays a crucial role in buffering volume changes and enabling structural reversibility and thus the $MoS_2$@rGO composite demonstrates improved rate capability and long-term stability, making it a promising candidate for advanced LIB anodes.

**j0021**

**Symmetric and Asymmetric Surface-Terminated MXenes as Low Diffusion Barrier Anode Materials for SIBs and PIBs**

Tuya Dey[a)], Bikash Chandra Gupta, Jagadish Chandra Mahato
*Department of Physics, Visva-Bharati, Santiniketan, 731235, West Bengal, India*
[a)]*tuyadey100@gmail.com*

Lithium-ion batteries (LIBs) have been the subject of extensive research over the past two decades. But because sodium and potassium are relatively abundant and lithium is scarce, research and development on sodium- and potassium-ion batteries (SIBs and PIBs) has attracted a lot of interest. Here we report the electronic, thermal, and mechanical properties of two-dimensional $Ti_2CFX$ (X =F, Cl, Br, and OH) monolayers and the adsorption-diffusion behavior of sodium and potassium atoms on these monolayers through density functional theory (DFT)-based calculations. Remarkably low diffusion barriers (in the range of 0.16–0.18 eV for Na, and 0.07–0.10 eV for K) on the $Ti_2CF_2$, $Ti_2CFCl$, $Ti_2CFBr$, and $Ti_2CFOH$ monolayers signify outstanding charge/discharge rate. Furthermore, the $Ti_2CFX$ (X =F, Cl, Br, and OH) MXenes exhibit theoretical storage capacities of 367.92 (367.92), 330.60 (330.60), 518.96 (259.48), and 559.58 (373.06) mAh/g for Na (K) with open circuit voltages of 0.39 (0.81), 0.31 (0.74), 0.30 (0.68), and 0.26 (0.55) V, respectively. Therefore, the $Ti_2CFX$ (X =F, Cl, Br, and OH) MXenes possess enormous potential for sodium-ion and potassium-ion batteries anode material.

**j0022**

**Strain-Engineered Band Convergence and Energy Filtering for Enhanced Thermoelectric Performance in Nb-Doped $SrTiO_3$ Thin Films**

Midhun Shah[1, 2 *], Jamshina Sanam.P.K [1], P.P.Pradyumnan[1]
[1] *Department of Physics, University of Calicut, Malappuram, Kerala-673635*
[2] *Department of Physics, Farook College, Kozhikode, Kerala -673632*
* *midhunshah@farookcollege.ac.in*

Achieving high thermoelectric power factors is essential for advancing efficient heat-to-electricity energy conversion technologies. In this work, we report a record-high power factor of 0.0185 $W/mK^2$ in $SrTi_{0.9}Nb_{0.1}O_{3-\delta}$ thin films deposited via RF magnetron sputtering under oxygen-deficient conditions. Comprehensive structural, compositional, and morphological analyses—carried out using XRD, XRF, SEM, and EDS—were systematically correlated with electrical and thermoelectric transport properties obtained from Hall and Seebeck measurements. High carrier concentrations ($10^{20}$–$10^{21}$ $cm^{-3}$) were primarily attributed to Nb substitution and oxygen vacancy formation, facilitated by pure argon sputtering and vacuum annealing. All samples exhibited behavior consistent with degenerate semiconductor transport, which could be effectively described using a parabolic band model. Notably, Seebeck coefficients ranging from 200–400 μV/K were achieved, driven by a synergy of energy filtering, modulation of effective mass, and strain-induced band degeneracy. These results highlight the critical role of controlled sputtering conditions in optimizing carrier dynamics and enhancing thermoelectric efficiency in perovskite oxide thin films.

**j0023**

**Development of 2D BP-$SrTiO_3$ Heterojunction Catalyst for Enhanced Electro(photo)catalysis**

Phulmani Basumatary and Anjalu Ramchiary*
*Department of Physics, Bodoland University, Rangalikhata, Kokrajhar, Assam, 783370, India.*
**Email: anjalu1417@buniv.edu.in; anjaluramchiary88@gmail.com*

Black phosphorus, exfoliated via atmospheric plasma-assisted synthesis and hydrothermally prepared SrTiO3 were integrated into a heterojunction (BP-STO) structure using a secondary hydrothermal process to explore its multifunctionality in energy-environmental applications. Extensive characterization unveiled the intricate physicochemical attributes, nuanced morphological and crystallographic structure, and tailored optoelectronic behavior of the composite. The BP-STO heterostructure demonstrated significantly improved efficiency in dye removal and electro(photo)-catalytic water splitting, underscoring its promise as a next-generation material for integrated energy conversion and environmental remediation technologies.

**j0024**

**Facile Synthesis and Electrochemical Evaluation of $Ni_{0.5}Co_{0.5}Fe_2O_4$ Nanospheres as Electrode Material for Supercapattery Applications**

P. Saha[1], D. Majumdar[2], R. Mondal[1, a)] and S. Kumar[1, a)]
[1]*Department of Physics, Jadavpur University, Kolkata-700032, India*
[2]*Department of Chemistry, Chandernagore College, Hooghly, WB-712136, India*
[a)] *Email: rituparnam.physics@jadavpuruniversity.in, kumar_dsa@yahoo.com*

$Ni_{0.5}Co_{0.5}Fe_2O_4$ (NC55) nanospheres (~ 80.73 nm) synthesized via a one-pot solvothermal method yield a cubic spinel ferrite ($Fd\bar{3}m$) with uniform morphology. The symmetric supercapattery device fabricated by using NC55 electrode material, exhibits excellent pseudocapacitive electrochemical behavior, including a high specific capacitance of ~71.53 $Fg^{-1}$, exceptional rate capability (47% retention at highest current), a maximum power density of ~1.58 $kWkg^{-1}$, and long-term cyclic stability with ~80% capacitance retention and ~77% coulombic efficiency over 1000 GCD cycles. These results emphasize the potential capability of NC55 nanospheres as a cost-effective, stable, and high-performance active electrode material for supercapattery applications.

**j0026**

**The X-ray Diffraction Study of Sol-Gel Derived NCM811 Material**

Vinod Singh[1], Sandeep Kumar[1], Weon Cheol Lim[2], Sangsul Lee[3,4], Keun Hwa Chae[2], and Jitendra Pal Singh[1, *]
[1]*Department of Sciences, Manav Rachna University, Faridabad, Haryana-121010, India*
[2]*Advanced Analysis and Data Center, Korea Institute of Science and Technology, Seoul-02792, Republic of Korea*
[3]*Pohang Accelerator Laboratory, POSTECH, Pohang-37673, Republic of Korea*
[4]*Department of Semiconductor Engineering, POSTECH, Pohang, Republic of Korea*
**Email: jpsingh@mru.edu.in*

In surge of high energy density cathode materials requirement for lithium-ion batteries (LiBs), $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ (NCM811) materials were synthesized from efficient and economic sol-gel method. This method utilizes metal nitrates as starting materials and citric acid as host. Precursor was formed after the stirring and subsequent drying at 110 °C. Initially, precursor was amorphous in the nature and remained in same phase after annealing at 300 °C. Annealing of precursor at 500 and 600 °C led to the formation of NCM811 with some minor impurity phases. At annealing temperature of 700, 800 and 900 °C pure crystalline phase of NCM811was obtained. On further annealing at 1000 °C, phase of NCM811 was observed to be deteriorated. Average Crystallite size estimated from the most intense peak of X-ray diffraction pattern, exhibited temperature-induced rise in crystallite size from 13 to 42 nm for 300 to 800 °C annealing temperatures. Thus, this method provided a way to control crystalline phase and crystallite size by controlling the annealing temperature given to the precursor.

**j0027**

**An Investigation of the Photoluminescence Properties of Europium Doped $MgSr_2(PO_4)_2$ Phosphor**

Neha Bharti[1], Rohit Mehra[1,a], Fouran Singh
[1] *Department of Physics, Dr B R Ambedkar National Institute of Technology* Jalandhar, Punjab-144008
[2] *Inter University Accelerator Centre, New Delhi-110067*
[a]*Corresponding Author Email: mehrar@nitj.ac.in*

This study investigates the photoluminescence characteristics of $Eu^3$-doped $MgSr_2(PO_4)_2$ phosphors synthesized by a high-temperature solid-state reaction. X-ray diffraction (XRD) analysis and Fourier transform infrared (FTIR) spectroscopy of the phosphor were done to get an understanding of the phosphor's crystalline structure and the bonding of its functional groups. Photoluminescence measurements showed a red emission under UV light, mainly because of the electric dipole transition $^5D_0 \rightarrow {}^7F_2$ of $Eu^{3+}$ ions. The spectral properties of $Eu^{3+}$ ions are in sites of the host lattice that lack an inversion center. The results show that this phosphor is structurally stable as well as optically active could be a strong candidate as a red phosphor in display and lighting applications.

**j0028**

**Theoretical Exploration of Structural, Mechanical and Electronic Properties of $MgScO_3$: A Full Potential Approach**

Meena Kumari[1], Shashank Nautiyal[2] and Shobha Kulshrestha[3]
*Department of Physics, School of Basic & Applied Sciences, Himachal Pradesh Technical University, Hamirpur (H.P.), India-17001*
*Department of Science, Mewar Institute of Management, Sector 4C, Vasundhra Ghaziabad, U.P., India-201012*
*NIMS University, Jaipur, Rajasthan*
**Email:meenaranot@gmail.com, shashank.fiziks.ju93@gmail.com, shobha011986@gmail.com*

In this communication, we have investigated structural, mechanical and electronic properties of Perovskite $MgScO_3$. We have used full potential linearized augmented plane wave method as implemented in Wien2k code. From our study we have been observed that $MgScO_3$ is mechanically ductile having anisotropic nature. From electronic band structure we found that the given compound is 100% spin polarized and exhibit half-metallic behaviour. The structural, mechanical and electronic properties have been reported for the first time. No experimental and theoretical data is available for comparison.

**j0029**

**Conductive Double Network Hydrogel for Functional Applications**

Ankush Kumar[1, a)] and Ajay D. Thakur[1]
[1]*Department of Physics IIT Patna, Bihta-801106, India*
[a)]*Corresponding author: ankush_2121ph18@iitp.ac.in*

In this study, a double-network (DN) hydrogel was synthesized using polyvinyl alcohol (PVA), sodium alginate (SA), and montmorillonite (MMT) for potential use in smart agriculture. The hydrogel was fabricated through a combination of physical and chemical crosslinking methods. Structural and crystallinity changes resulting from MMT incorporation were confirmed using X-

ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR). The hydrogel's performance was assessed through measurements of electrical conductivity, tensile strength, and water retention capacity. The DN hydrogel demonstrated improved tensile strength, electrical conductivity, and moderate water retention property, indicating enhanced mechanical stability and facilitated ionic transport due to the uniform dispersion of MMT.

**j0032**

**On the structural study of Si-based pre-lithiated anode synthesized by melt solidification method and impact of environmental conditions**

Ashish Kumar Mishra, Anjali, Monika and Balbir Singh Patial*
*Department of Physics, Himachal Pradesh University, Summerhill, Shimla, Himachal Pradesh, 171005, INDIA.*
**bspatial@gmail.com*

Lithium-ion batteries are critical for advancing energy storage, necessitating anode materials with enhanced energy density and cycling stability to meet escalating demands in portable electronics and renewable energy systems. Si is a promising anode material due to its high theoretical specific capacity (~4199 mAh/g for the $Li_{21}Si_5$ phase), nearly tenfold that of graphite (~372 mAh/g). However, silicon's practical application is hindered by significant volume expansion (~300%) during lithiation, leading to mechanical degradation and active lithium loss. Pre-lithiation of silicon anodes offers a potential solution to mitigate lithium loss and to improve electrochemical performance. This study investigates the synthesis of the $Li_{21}Si_5$ phase via melt solidification process under ambient air and inert atmospheres. The synthesized materials were characterized using X-ray diffraction, scanning electron microscopy, energy-dispersive X-ray spectroscopy, and X-ray photoelectron spectroscopy to evaluate phase purity, structural integrity, and chemical composition. Results provide insights into the impact of synthesis conditions on $Li_{21}Si_5$.

**j0033**

**Thin Film CuO and $MnO_2$/CuO On Cu Foil For Supercapacitor Application**

Neha Phadte and RajeshKumar Shankar Hyam*
*School of Physical and Applied Sciences, Goa University, Goa, India, 403206*
**Corresponding author email: rajesh.hyam@unigoa.ac.in*

The selection and design of electrode materials are critical in defining the performance of supercapacitors. The surface area, film thickness, number of oxidation states, and stability are all important factors responsible for good results. In this study, CuO nanoneedles and layered heterostructure of $MnO_2$ and CuO were electrochemically prepared on a Cu foil. The structure, and morphology was determined by Raman Spectroscopy and Scanning Electron Microscopy respectively. A mixed stoichiometric form of $MnO_2$ and $Mn_2O_3$ was observed for the heterostructure. Cyclic Voltammetry and Galvanostatic charge Discharge was performed to understand the electrochemical nature of the samples. The CuO_Cu exhibited a specific capacitance of 218 F $g^{-1}$, while the $MnO_2$/$Mn_2O_3$_Cu electrode achieved a higher value of 454 F $g^{-1}$ at a scan rate of 20 mV $s^{-1}$ in 1 M KOH electrolyte.

**j0034**

**Synergistic $MoSe_2$-CuO Heterointerfaces for Enzyme-Free Glucose Monitoring**

Rashbihari Layek[1] and Pathik Kumbhakar[1]
*[1]Department of Physics, National Institute of Technology Durgapur, Durgapur-713209, West Bengal, India*
**Email: rl.22ph1104@phd.nitdgp.ac.in*

The design of efficient non-enzymatic glucose sensors is crucial to address the drawbacks of enzymatic systems, which often suffer from instability and limited operational conditions. Herein, the $MoSe_2$-CuO nanocomposites have been prepared to serve as a highly efficient electrocatalyst for glucose sensing. The integration of two-dimensional $MoSe_2$ with CuO nanoparticles facilitates strong interfacial coupling, rapid electron transfer, and abundant electroactive sites, leading to superior electrocatalytic activity toward glucose oxidation. The fabricated sensor exhibits a rapid response time of 3 s, a low detection limit of 0.5 μM with sensitivity of 123 μA $mM^{-1}$ $cm^{-2}$ and a wide linear detection range. Furthermore, its applicability is successfully demonstrated in real sample analysis using fruit juice.

**j0036**

**Comparative Evaluation of $Co_3O_4$ and $CoSeO_3$ Electrocatalysts for Aluminum-Air Batteries**

Shraddha M. Rajore[1], Archana R. Kanwade[1], Parasharam M. Shirage[1]*
*[1]Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Indore, Simrol-453552, Indore, MP, India.*
**Corresponding author: pmshirage@iiti.ac.in; paras.shirage@gmail.com*

Aluminum-air batteries (AABs) are emerging as high energy density energy storage systems, utilizing aluminum as the anode and ambient air as the cathode. This study presents a comparative evaluation of $Co_3O_4$ and cobalt selenium oxide $CoSeO_3$ as electrocatalysts for enhancement of the electrochemical performance of AAB. Structural and morphological characteristics were examined using XRD and SEM, while elemental distribution was confirmed through additional physicochemical analyses. Electrochemical properties were evaluated using linear sweep voltammetry (LSV), and chronoamperometry. Battery performance was evaluated using galvanostatic charge-discharge (GCD). The results reveal distinct differences in catalytic activity and stability between $Co_3O_4$ and $CoSeO_3$, highlighting the critical role of catalyst selection in optimizing AAB efficiency. This work contributes to the advancement of sustainable and high-performance energy storage technologies.

**j0038**

**Fabrication of Bimetallic Ni-Co BMOF with varying ratios for Photocatalysis Applications**

Meera Antony[1] , P. Thangadurai[1, *]

*Centre for Nanoscience and Technology, Pondicherry University, Kalapet, Puducherry- 605014, India*

**Email: thangaduraip.nst@pondiuni.edu.in / thangadurai.p@gmail.com*

A bimetallic metal-organic framework (BMOF) material containing Ni and Co as metals and terephthalic acid as ligand, with varying ratios of the metals, were synthesized by a one-pot solvothermal method. The Ni: Co ratio was varied as 1:1,1:3,1:5 Ni-Co BMOFs. They were formed with a good crystalline phase as observed by X-ray diffraction and Raman scattering experiments. Elemental analysis by X-ray photoelectron spectroscopy shows the presence of Ni, Co, C and O. The band gap of the MOF varied from 2.3 eV to 2.9 eV. They showed a good absorption in the visible light region, and therefore, it is active in degrading the Congo red dye under visible light irradiation. The degradation of CR dye varied with changing the metal ratio in the BMOF, with the maximum degradation of 94.9% CR dye shown by the 1:5 Ni: Co in the BMOF.

**j0039**

**Phase Evolution And Environmental Remediation Properties Of $Zn_3V_2O_8$ Derived From A Hydrated Precursor**

Karthigeswaramoorthi. V[1] and P. Thangadurai[1, a)]

*Centre for Nanoscience and Technology, Pondicherry University, Kalapet, Puducherry- 605014, India*

**Email: thangaduraip.nst@pondiuni.edu.in / thangadurai.p@gmail.com*

Zinc vanadate, a semiconducting metal oxide, was prepared by a coprecipitation method followed by calcination at 600 °C with the stoichiometry $Zn_3V_2O_8$. The crystal structure was confirmed to be orthorhombic using X-ray diffraction. Further structural confirmation was obtained from Raman spectroscopy. The elemental composition was analyzed using X-ray photoelectron spectroscopy. The optical bandgap was found to be 3.06 eV, making the material suitable for photocatalytic applications. $Zn_3V_2O_8$ exhibited excellent photocatalytic performance by degrading Methylene Blue dye under UV light irradiation with an efficiency of 99.71%.

**j0040**

**Sol-Gel Processed BCZT Thin Films for Energy Storage Applications**

Satyabrata Lenka[1], Suresh Kumar Garlapati[2,b)] , Mahesh Peddigari[1, a)]

*1Functional Ceramics Laboratory, Department of Physics, Indian Institute of Technology Hyderabad, Telangana, India-502285*

*2Department of Materials Science and Metallurgical Engineering, Indian Institute of Technology Hyderabad, Telangana, India-502285*

*a)Corresponding author: mahesh.p@phy.iith.ac.in*

*b)Corresponding author: gsuresh@msme.iith.ac.in*

Dielectric ceramic capacitors, which store electric energy via electrostatic polarisation, can be used in pulsed power applications due to their ultra-short charge and discharge cycles. Moreover, due to compact and defect-free microstructures, ceramic films can sustain higher electric fields and display higher energy storage densities than their bulk counterparts. Our current initiatives focus on lead-free barium titanate–based (BTO) compounds due to their superior energy storage properties. With the help of the sol-gel method, $(Ba_{0.85}Ca_{0.15}Zr_{0.10}Ti_{0.90})O_3$ (BCZT) thin films have been spin-coated on Pt/Si substrates. The effect of solution concentration, deposition and annealing conditions has been optimised to improve the film microstructures. Stoichiometry was modified to optimise the material properties for fabricating energy storage capacitors to enhance their performance and efficiency. The present work will contribute towards creating efficient energy storage devices for future electronic systems.

**j0041**

**Preparation and Characterization of 2H Phase $MoS_2$ Based Room Temperature Ammonia**

Hiritika* and Aman Mahajan

*Department of Physics, Guru Nanak Dev University, Amritsar 143005, India*

**hiritikakoundal5@gmail.com*

Ammonia ($NH_3$) is a critical biomarker in human health as well as a very dangerous pollutant causing various respiratory disorders and environment degradation. Till date, metal oxides based gas sensors are widely used to detect $NH_3$, however, they require high operating temperature (~200°C to 400°C). To overcome this problem, we have synthesized hexagonal (2H) phase molybdenum disulfide ($MoS_2$) via the hydrothermal method to fabricate a chemiresistive sensor, which can operate at room temperature. The X-Ray diffraction and Raman spectroscopy studies confirmed the formation of the as synthesized 2H $MoS_2$ and the fabricated sensor displayed an excellent selectivity towards $NH_3$ amongst other gases like ethanol, methanol and hydrogen peroxide with a response of 22.13% for 20 ppm $NH_3$ and response/recovery time of 175.64s/120s. Also, with increase in the concentration of $NH_3$, the response value was seen to increase from 25.2% (40 ppm) to 50.9% (100 ppm).

**j0043**

**ZnO/MWCNT Nanocomposite Based Chemiresistive DMC Sensing for Monitoring Thermal Runaway**

Arshiya Wadhwa[1, (a)], Aman Mahajan[1]

[1]*Department of Physics, Guru Nanak Dev University, Amritsar 143005, India*
[a)]*Corresponding author: arshiyawadhwa125@gmail.com*
This study reports the design and characterization of a chemiresistive gas sensor for selective detection of dimethyl carbonate (DMC), a volatile organic compound associated with lithium-ion battery failure. Zinc Oxide (ZnO) nanoparticles were synthesized via co-precipitation method, while multi-walled carbon nanotubes (MWCNT) were acid-functionalized to enhance its interfacial interactions. The sensor fabricated by the ZnO/MWCNT nanocomposite demonstrated a significant response towards low concentrations of DMC (75- 150 ppm), with fast response and recovery times (95 s/15 s). This enhanced sensitivity is attributed to the synergistic effect arising from the interfacial interaction between ZnO and MWCNT, resulting in improved charge transfer and increased number of active sites, thereby highlighting its potential to be integrated into advanced gas sensing systems for environmental and battery safety applications.

**j0044**

**Surface Engineering of $Ti_3C_2T_x$ MXene using Functionalized MWCNT for Supercapacitor Application**

Akshidha Singla[1], Aman Mahajan[1, a)] and Rajnish Dhiman[2]
[1]*Department of Physics, Guru Nanak Dev University Amritsar, Punjab, India-143005*
[2]*Department of Physics, Malaviya national Institute of Technology, Jaipur, India -302017*
[a]*Email:aman.phy@gndu.ac.in*
Supercapacitor (SC), an advanced and green technology in the field of energy storage; capable of storing charges efficiently, suffer from certain intrinsic limitations which impede their scalability. Accordingly, herein, a novel two-dimensional $Ti_3C_2T_x$ MXene was employed as electrode in SC by virtue of large surface area, high conductivity and tunable surface chemistry. Further, incorporation of MWCNT-COOH in MXene enhances the facile charge transfer mechanism via hydrogen bonding and electrostatic interaction of COOH group with surface functionalities of MXene. The electrochemical performance of $Ti_3C_2T_x$/MWCNT-COOH based SCs was meticulously investigated using cyclic voltammetry, galvanostatic charge-discharge and electrochemical impedance spectroscopy, exhibited maximum specific capacitance of 417.8 $Fg^{-1}$ at current density of 0.3 $Ag^{-1}$, delivers high energy density of 130.56 Wh $kg^{-1}$ and power density of 4.5 kW $kg^{-1}$, even shows good capacitance retention of 93.33% capacitance after 5000 cycles respectively.

**j0046**

**Electrooxidation of Ethylene Glycol by Au-Ag/C Nano catalyst For Fuel Cell Applications**

Bholanath Mahato, Santanu Dey and Soumen Basu
*National Institute of Technology Durgapur, Durgapur, 713209, West Bengal, India.*
**Email: bm.24ph1104@nitdgp.ac.in*
In this work, we have synthesized Au/C and $Au_{60}Ag_{40}$/C (20 wt% metal loading on carbon support) bimetallic electrocatalyst with the help of wet chemical synthesis technique. To know about the crystalline structure, surface morphology, we have been employed X-ray diffraction spectroscopy (XRD), Field emission scanning electron microscopy (FESEM) respectively. To investigate about electrochemical performances of the as prepared electrocatalysts, we have implemented Cyclic Voltammetry (CV), Electrochemical impedance spectroscopy (EIS) and Chronoamperometry (CA) measurements. The as-synthesized nano catalyst shows excellent electrocatalytic activities as anode catalyst for ethylene glycol ($C_2H_6O_2$) electro oxidation in alkaline medium. Our catalyst has also been shown better performances than commercial traditional Au/C catalyst and can be successfully utilized for alkaline ethylene glycol-based fuel cell applications.

**j0047**

**Effect of Manganese Doping on the Electrochemical Behaviour of $V_2O_5$ for Energy Storage Applications**

Prashant[1], Abhishek Kumar[1], Neha Kondal[1, a)]
[1]*Department of Physics, Chandigarh University, Gharuan, Mohali, Punjab 140413, India*
[a)]*Corresponding author: nehakondal91@gmail.com*
This study investigates the influence of 4% Mn doping on the structural, morphological, and electrochemical properties of vanadium pentoxide ($V_2O_5$) for energy storage applications. The synthesized Mn-doped $V_2O_5$ ($V_{1.96}Mn_{0.04}O_5$) exhibited an orthorhombic crystalline structure confirmed by XRD, with increased grain size and lattice strain compared to pristine $V_2O_5$. BET analysis revealed enhanced porosity and surface area in the doped sample, while FESEM images showed morphological modifications supportive of higher electrochemical activity. Electrochemical studies using cyclic voltammetry demonstrated improved capacitive performance for the doped sample, with diffusion-controlled charge storage behavior. The Mn doping was found to enhance Li-ion diffusion and reduce impedance, positioning $V_{1.96}Mn_{0.04}O_5$ as a promising cathode material for lithium-ion battery systems.

**j0048**

**Upconversion Study of $Er^{+3}$, $Er^{+3}/Dy^{+3}$, $Er^{+3}/Yb^{+3}$ in tellurite tungstate glass for enhanced a-Si solar cells photocurrent**

Sakshi Desai[1] and *Reshma Raut Dessai[2]
[1] *School of Physical and Applied Sciences, Goa University, Taleigao Plateau, Goa, 403206, India*
**Email: reshma@unigoa.ac.in )*

The present study reports the influence of $Er^{3+}$, $Er^{3+}$-$Dy^{3+}$, and $Er^{3+}$-$Yb^{3+}$ doping on the upconversion emission intensity of $TeO_2$-$WO_3$-$ZrO_2$ glasses synthesized by melt-quenching technique. The amorphous nature of the glasses has been confirmed from the XRD analysis. The absorbance behavior and Upconversion emission intensity have been explained from the pump power-based analysis. The color purity and color-tunability have been analyzed by the CIE chromaticity diagram. When coupled to an a-Si solar cell, $Er^{+3}$ and $Er^{+3}$-$Yb^{+3}$ doped glasses significantly increased photocurrent under 980 nm excitation, demonstrating their potential for spectral conversion for photovoltaic applications.

**j0049**

**Synthesis and Characterization of Tungsten Doped Barium Vanadate Glasses for Application in Energy Storage Devices**

Kriti[1], Divya Mahajan[1], Renuka C[2] and Atul Khanna[1,a)]
[1]*Sensors and Glass Physics Laboratory, Department of Physics, Guru Nanak Dev University, Amristar-143005, Punjab, India*
[2]*Department of Physics, Global Academy of Technology, R.R Nagar, Bengaluru-5600098, Karanatka*
[a)]*Corresponding Author :atul.phy@gndu.ac.in*

Barium vanadate glasses with and without tungsten are prepared by splat quenching technique in the temperature range : 700-800˚C and are characterized using X-ray diffraction (XRD), Raman spectroscopy, differential scanning calorimetery and cyclic voltammetry. The XRD studies confirm the amorphous nature of all the glass samples. Raman spectra show a sharp boson peak at low frequency ~55 $cm^{-1}$, which is a characteristic feature of glasses. Raman bands centered at 664 $cm^{-1}$ are due to the stretching mode of doubly coordinated oxygen ($V_2$-O) and the peak at 894 $cm^{-1}$ is due to the symmetric stretching mode of O–V–O bonds. The glass transition temperature ($T_g$) of barium vanadate samples is in the range: 255 -282˚C. The specific capacitance of barium vanadate samples with and without tungsten is in the range: 10.03-61.5 $Fkg^{-1}$.

**j0050**

**$(FeCoCrMnZn)_3O_4$ High Entropy Oxide as Anode for Li ion Battery: Dependence on Synthesis Process**

Sidhartha Sankar Sahoo*, Chandrani Nayak, Seemita Banerjee, Himashu Srivastava, Dibyendu Bhattacahryya
*Atomic and Molecular Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, India.*
**Email: sahooss@barc.gov.in*

$(FeCoCrMnZn)_3O_4$ high entropy oxide samples were prepared through solid state synthesis route involving two major steps viz., ball milling and annealing. One sample (HEO1) was prepared via 12 hrs. of ball milling and 5 hrs. of air annealing at 1000ºC, while the other sample (HEO2) was prepared via 3 hrs. of ball milling and 12 hrs. of air annealing at 1000ºC. Structural and morphological analysis of both the samples were done by XRD, HRTEM, SAED and EDS. Lithium-ion half cells were prepared using both the samples as anodes and battery performances were tested by galvanostatic charge-discharge (GCD) measurements. It has been found that the HEO sample prepared with shorter ball milling and longer annealing (HEO2) shows better cycle performance as anode of Li ion battery at high current than that prepared with longer ball milling and shorter annealing (HEO1).

**j0051**

**Synthesis and Characterization of Monovalent and Divalent Ion Doped Vanadium Tellurite Glasses for Applications in Energy Storage Devices**

Rohit Kumar Kasaudhan[1], Kajal Dadwal[1], Sunita[1], Satpal Kaur[1], Renuka C[2], Atul Khanna[1,a)]
[1)] *Department of Physics, Guru Nanak Dev University, Amritsar-143005, Punjab, India*
[2)] *Department of Physics, Global Academy of Technology, R R Nagar, Bengaluru-560098*
[a)]*Corresponding author: atul.phy@gndu.ac.in*

In this study, vanadium tellurite glasses of composition $50V_2O_5$-$45TeO_2$-$5M_2O$/RO where (M=Na, and R=Zn, Ba and Sr) are prepared using the melt quenching technique and characterized by X-ray diffraction(XRD), Raman spectroscopy, two probe electrical conductivity and the electrochemical properties of the glass cathode materials were investigated by cyclic voltammetry (CV) studies. XRD studies confirmed the amorphous nature of the samples. The temperature dependent electrical conductivity measurements were done by using the two-probe setup. The room temperature dc electrical conductivity of the samples is in the range of $10^{-4}$-$10^{-2}$ $mS{\cdot}cm^{-1}$ and increases with increase in temperature, whereas the values of activation energy are in the range of 0.3-0.37eV for the samples. CV studies show that the specific capacitance ($C_p$) is in the range of 44-121 $F{\cdot}kg^{-1}$.

**j0052**

**rGO Enhanced $SnO_2$ Photocatalysts for Efficient Photocatalytic Degradation of Antibiotics**

K.Nithya[1],Jayapandi Selvam[2] , K.Kaviya[1], M. Tamilelakkiya[1*]
[1]*Department of Physics,Thiagarajar College of Engineering, Madurai, Tamil Nadu,625015,India*
[2]*Energy and Environmental Remediation Laboratory, Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur, Chennai 603 203, Tamil Nadu, India*
**Corresponding Author Email Id: mtphy@tce.edu*

The growing presence of pharmaceutical residues in our aquatic environments and their potential risk to human health is not a simple problem to solve. Antibiotics are among the most persistent of all pharmaceuticals. Nitrofurantoin is a widely used pharmaceutical that is often detected in aquatic environments, itisalsoable to resist a wide variety of methods commonly used to treat water so that its removal is more challenging. A visible-light-active photocatalyst was designed that was based upon $SnO_2$ fused combined with reduced graphene oxide (rGO). Thecatalystimproves light utilization,strengthens charge recombination,

andimproves photocatalytic activity. Under natural sunlight, the optimized $SnO_2$/rGO catalyst achieved over 92% degradation of nitrofurantoin from aqueous solution.The improved performance is due to enhanced charge transfer mechanism that increases the generation of reactive oxygen species. This hasprovided an effective and sustainable route for removing persistent antibiotics from contaminated water.

**j0054**

**Comparative Study for Shape Stability of Paraffin/SEBS and Paraffin/polyaniline Composites**

Sheetal[1], Deepika P. Joshi[1, a)], Pankaj Singh Rawat[1], Jaspreet Singh Aulakh[2] and Neetu Bora[3]

*[1]Department of Physics, G.B. Pant University of Agriculture and Technology, Pantnagar, India, 263145.[2]Department of Applied Sciences (Physics), G. L. Bajaj Institute of Technology and Management, Greater Noida, Uttar Pradesh, 231306.[3]Indian Institute of Science, Bangalore, 560012.*

*[a)]Corresponding author:Deepikapjoshi.bpp@gbpuat.ac.in*

Leakage during phase transitions of phase change materials (PCMs) is a critical issue that hinders their utility in practical applications. Therefore, shape stabilization of PCMs becomes essential to address this challenge. In the present work, an attempt has been made to investigate the shape stability of paraffin wax (melting point: 58–60 °C) by incorporating two different supporting materials: polyaniline and SEBS (styrene-ethylene-butylene-styrene).X-ray diffraction (XRD) has confirmed the successful synthesis of both polyaniline- and SEBS-based composite PCMs. A leakage test is carried out at 70 °C for more than 500 thermal cycles with 30 min cycle each, to investigate the shape stability of the composite PCMs.The leakage test has demonstrated that SPCM2 (20 wt% SEBS) and PPCM2 (20 wt% polyaniline) have exhibited excellent shape stability. The maximum leakage in SPCM2 and PPCM2 was found to be 0.2–0.3% and 0.08%, respectively. Lower leakage observed in PPCM2.In conclusion, PPCM2 demonstrated superior shape stability and can be an effective material for thermal energy storage applications.

**j0055**

**Enhanced Supercapacitor Performance Through Lithium Substitution In Nickel Ferrite**

Manjeet Jakhar[1] and Kanhaiya Lal Yadav[1, 2, a)]

*[1]Smart Materials Research Laboratory, Department of Physics, Indian Institute of Technology Roorkee, Uttarakhand, India-247667*

*[2]Centre for Sustainable Energy, Indian Institute of Technology Roorkee, Uttarakhand, India-247667*

**manjeet1@ph.iitr.ac.in*

Sustainable energy systems require efficient storage to manage renewable intermittency; supercapacitors offer fast charging and high-power delivery. This study highlights the impact of lithium substitution on the electrochemical properties of nickel ferrite. X-ray diffraction analysis confirmed the cubic spinel crystalline structure. Electrochemical measurements were carried out with a three-electrode setup in a 6 M KOH electrolyte solution. The GCD measurements show a notable increase in specific capacitance, rising from 156 F/g to 534 F/g upon the lithium substitution. These findings imply that doping nickel ferrite with lithium improves the material's electrochemical characteristics, positioning it as a promising candidate for supercapacitor electrodes.

**j0056**

**Facile Synthesis of Ammonium Jarosite for Cost-Effective and Stable Oxygen Evolution Catalysis**

Haripal Singh Dhayal[1], Nishad G. Deshpande[1]*

*1 Department of Applied Science & Humanities, Indian Institute of Information Technology Surat, Kholwad Campus, Kamrej, Surat 394185, Gujarat, India*

**Email: nishad.deshpande@iiitsurat.ac.in (Email of corresponding author)*

In this study, ammonium jarosite thin films were fabricated on flexible stainless steel (SS) substrates using a simple, low-cost chemical bath deposition (CBD) method. XRD and Raman spectroscopy confirmed the formation of crystalline ammonium jarosite. The films' electrocatalytic activity for the oxygen evolution reaction (OER) in alkaline conditions was evaluated against bare SS. The ammonium jarosite films showed significantly improved catalytic performance, with enhanced reaction kinetics and a higher density of active sites. At 10 mA/cm², they required a lower overpotential of 421 mV, compared to 670 mV for SS, and exhibited a Tafel slope of 113 mV/dec, indicating better charge transfer than SS (250 mV/dec). These results highlight ammonium jarosite as an efficient, low-cost OER electrocatalyst with strong potential for scalable, sustainable water-splitting applications.

**j0059**

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

Arpita Singha[1 a], Saket Asthana[1]

*[1] Advanced Functional Materials Laboratory, Department of Physics, Indian Institute of Technology Hyderabad, Kandi, Sangareddy 502284, Telangana, India*

*[a)] Corresponding author: arpitasingha.8895@gmail.com*

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.

**j0061**

**Insights Into 2D Rubidium Bismuth Iodide Perovskite Towards Optoelectronic Applications**

Shruti Shah[1,2], Sandesh Jadkar[1,2*]
[1]*Center for energy studies, Savitribai Phule Pune University*
[2]*Department of Physics, Savitribai Phule Pune University*
[*]*Email: sandesh@physics.unipune.ac.in*

Now-a-days, perovskites are emerged as the new building blocks for optoelectronic applications. Here in, we have synthesized the all inorganic stoichiometric Rubidium Bismuth Iodide ($Rb_3Bi_2I_9$) abbreviated as RBI perovskite by sequential spin coating method for opto-electronic applications. It is expected that the replacement of bigger "A" cation with smaller cation will change the dimer structure into 2D layered structure that will enhance the charge transport. The confirmed structure from XRD analysis is monoclinic lattice structure with space group $P2_1/n$. The bandgap obtained from UV-Vis spectra is ~2 eV with absorption coefficient in the range of $10^5$ $cm^{-1}$. The morphology is uniform and covered with disc shaped RBI grains. The fabricated photodetector device shows sharp response (~ 150 ms) and recovery times (~ 45 ms) honoring RBI as a potential material for Optoelectronic applications. The stable performance is an outcome of straddled band alignment between the individual layers of devices.

**j0064**

**Investigation of the solubility limit of Mg in $Mg_3Sb_2$ to synthesize n-type zintl compound for the fabrication of efficient room temperature thermoelectric power generator**

Swadesh Mohanty, Ranita Basu*
*Technical Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, India.*
**Email: ranitab@barc.gov.in*

The widespread availability of room to mid temperature waste heat has spurred interest in efficient thermoelectric materials in this range. Although $Bi_2Te_3$ remains as one of the most efficient and commercially available mid temperature thermoelectric materials, what leaves a question mark is the toxicity of its constituents. In recent years, $Mg_3Sb_2$ has come up as a promising room to mid temperature alternative to $Bi_2Te_3$ showing remarkable room temperature performance, high thermal stability, and high structural toughness. Also, the constituents are nontoxic and has a higher abundance in nature. However, the intrinsic p-type $Mg_3Sb_2$ has low carrier concentration, making it an unreliable choice. This can be averted by adding excess amount of Mg during the synthesis of the alloy. Here in this study, we have attempted to determine the solubility limit of excess Mg, as too high Mg during synthesis may lead to the formation of Mg-rich secondary precipitate and may alter the chemistry of the alloy. Eventually, the idea of compensating the loss of Mg during synthesis will not be served. Thus, series of samples with varying compositions were synthesized and analysed to arrive at the solubility limit of Mg in $Mg_3Sb_2$ which will consequently have superior thermoelectric performance.

**j0065**

**Structural and Electrochemical Investigation of Dendritic-Fibrous $CeO_2$/a-rGO Edifices for Smart Supercapacitors**

Shruti Rialach[1,2,a)] and Surinder Paul[1]
[1]*Department of Physics and Astronomical Science, Central University of Himachal Pradesh, Dharamshala-176215*
[2]*Department of Applied Science, CGC College of Engineering, Chandigarh Group of Colleges, Landran, Mohali-140307*
[a)]*shruti.rialach@gmail.com*

With the escalating demand for high-performance energy storage systems, the development of advanced electrode materials with enhanced conductivity and redox activity has become essential. In response to the growing need for efficient and durable energy storage materials, this study presents the synthesis and detailed characterization of dendritic fibrous $CeO_2$/amorphous-reduced graphene oxide ($CeO_2$/a-rGO) composites. The material was derived through pyrolysis of cerium-based metal-organic frameworks (Ce-MOFs) integrated with graphene oxide, using an organic ligand-assisted solvothermal approach followed by thermal treatment at 500 °C. Structural analysis via Rietveld-refined X-ray diffraction confirmed the formation of nanocrystalline fluorite-phase $CeO_2$ with an average crystallite size of 8.28 nm. The amorphous nature of the rGO matrix was validated through high-resolution XPS of the C 1s region, revealing characteristic oxygen functionalities and the absence of π-π* satellite peaks. HR-TEM images showed uniform dispersion of dendritic fibrous $CeO_2$ nanocrystallites within the a-rGO framework. Electrochemical measurements conducted in a three-electrode system demonstrated excellent performance, with the $CeO_2$/a-rGO composite achieving a specific capacitance of 1190.58 F $g^{-1}$ at 1 A $g^{-1}$ and an energy density of 382.60 Wh $kg^{-1}$ at a power density of 4.00 kW $kg^{-1}$. These results underscore the potential of $CeO_2$/a-rGO as a high-performance electrode material for next-generation smart supercapacitors, offering superior charge storage, structural robustness, and long-term cycling stability.

**j0066**

**First Principles Calculations For Hydrogen Storage Over Two-dimensional Materials**

Sulagna Ghosh[1, 2]*, Jabed Aktar Khan[1, 2], Palash Nath[3] and Dirtha Sanyal[1, 2]
[1]*Variable Energy Cyclotron Centre, 1/AF, Bidhannagar, Kolkata – 700064, India*

[2]*Homi Bhabha National Institute, Anushakti Nagar, Mumbai – 400094, India*
[3]*Department of Physics, Ramakrishna Mission Vivekananda Centenary College, Rahara, Kolkata – 700118, India*
**Email: sulagna.ghosh97@gmail.com (Email of corresponding author)*
Monolayer materials possess a large surface area and tunable functional properties, which can be excellent for application in gas sensing and storage. In our work, van der Waals density functional theory (vdW-DFT) and kinetic Monte-Carlo (kMC) simulation have been jointly used to study the dynamics of $H_2$ molecules over four different monolayers: ZnO, BN, $SnS_2$ and $GeO_2$. During the adsorption, the repulsive interaction between two molecules plays a key role to determine the maximum number of $H_2$ that can be packed inside one unit cell of the monolayer. Out of the four materials, hexagonal BN can achieve the maximum $H_2$ gravimetric density of 7.5% weight percentage (wt%). With an adsorption energy of about −68 meV, the surface coverage of $H_2$ molecules can become close to 1.0 at 1.0 atmospheric pressure and below 100 K temperature. In this case, the $H_2$ adsorption energy can be further increased by formation of point defects, such as vacancy, or carbon substitution. Further, our study also shows that carbon cluster formation over monolayer BN substrate can elevate the $H_2$ adsorption energy to −84 meV, making it more beneficial for practical storage applications.

**j0067**
**Understanding of the non-linear variation in the optical band gap of $Ni_{1-x}Co_xO$ ($0 \le x \le 1$) solid solution through electronic structure analysis**
Kiran Baraik[1, 2, *], Velaga Srihari[3], Rakesh Kumar[1], A. K. Yadav[4], Rajiv Kamparath[5], Mukul Gupta[6], Pragya Tiwari[1], S. D. Singh[1, 2], Tapas Ganguli[1, 2]
[1]*Accelerator Physics and Synchrotrons Utilization Division, Raja Ramanna Centre for Advanced Technology, Indore-452013, India*
[2]*Homi Bhabha National Institute, Anushakti Nagar, Mumbai-400094, India*
[3]*High Pressure and Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, India*
[4]*Atomic and Molecular Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, India*
[5]*High Energy Lasers & Optics Division, Raja Ramanna Centre for Advanced Technology, Indore-452013, India*
[6]*UGC-DAE-Consortium for Scientific Research, Indore-452001, India*
**Email: kiranb@rrcat.gov.in*
Non-linear variation of optical band gap of NiO solid solution upon Co substitution in the complete composition range has been investigated from electronic structure study of unoccupied (conduction band) and occupied (valence band) states using X-ray absorption spectroscopy (XAS) at oxygen K-edge and photoelectron spectroscopy (PES) at the beamlines of Indus-2 synchrotron radiation facility, respectively. The non-linear variation of the optical band gap is attributed to the non-linear shift in the conduction band (CB) edge due to Co substitution in NiO. The optical band gap variation has negligible contribution from the valence band (VB) edge upon Co substitution. Both the CB and VB are found to be dominated by the localized Ni 3d orbitals. Resonant PES studies at Ni and Co 2p to 3d absorption threshold identify distinct Ni and Co derived states in the VB, confirming the charge-transfer insulating nature of the solid solution. The core level PES and X-ray absorption near edge structure (XANE) studies at Ni and Co K-edges confirm the presence of Ni and Co ions in +2 oxidation state, completely ruling out the possibility of change in the optical band in this system due to change in the oxidation state of Ni and Co.

**j0068**
**Exploring the Effect of Exfoliated Graphite Incorporation in $CrCo_2O_4$ Electrodes for Advanced Supercapacitors**
Amardeep Narwal[1, a], Kanhaiya Lal Yadav[1,2]
[1]*Smart Material Research Laboratory, Department of Physics, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand 247667, India*
[2] *Centre for Sustainable Energy, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand 247667, India*
**Email: amardeep@ph.iitr.ac.in)*
The pursuit of high-performance supercapacitor electrodes has driven research into advanced composite materials that integrate the advantages of metal oxides with conductive carbonaceous components. In this study, we explore the impact of exfoliated graphite incorporation into chromium cobalt oxide ($CrCo_2O_4$) electrodes synthesized via a simple co-precipitation method for application in advanced aqueous supercapacitors. Pristine $CrCo_2O_4$ demonstrated a specific capacitance of 90 F $g^{-1}$ at 0.5 $Ag^{-1}$, which significantly increased to 204 F $g^{-1}$ upon compositing with 1 wt% exfoliated graphite. The enhancement is attributed to the synergistic effects arising from the conductive network of exfoliated graphite and the pseudocapacitive nature of $CrCo_2O_4$, leading to improved charge transport and greater electrochemical surface area. Moreover, the composite electrode exhibited excellent cycling stability, maintaining 90% coulombic efficiency and 79% capacitance retention after 5,000 charge-discharge cycles. These results underscore the effectiveness of exfoliated graphite as an additive to boost the electrochemical performance and operational longevity of metal oxide-based supercapacitor electrodes.

**j0069**
**Synergistic Co-doping Fe and W Driven Hierarchical Nanoflakes Morphology for Enhanced Electrochromic Performance in $V_2O_5$**
Akanksha Malik[1]*, Richa Saini[1], Anshu Singh[1] Thanigai Arul Kumaravelu[2], Asokan Kandasami[3], and C.L. Dong[2]

[1]*Department of Physics, Kanya Gurukul Campus, Gurukul Kangri (Deemed to be University), Haridwar, Uttrakhand-249404, India*
[2]*Department of Physics, Tamkang University, Tamsui 25137, Taiwan*
[3]*Department of Physics & Centre for Interdisciplinary Research, University of Petroleum and Energy Studies (UPES), Dehradun, Uttarakhand-248007, India.*
*Email: malik.akanksha08@gmail.com**
This study focuses on the synergistic impact of co-doping of Fe and W dopants-induced structural, morphological, and electronic alterations on electrochromic performance. The XRD spectra reveal that the co-doping of Fe and W in $V_2O_5$ caused a decrease in crystallite size with a peak broadening. The vibrational modes of the samples were investigated using Raman spectroscopy. The higher charge mobility was correlated with improved optical transmittance spectra around 10 % increases as compared to pristine. Changes in the oxidation state of vanadium and increased oxygen vacancies in the co-doped sample were confirmed by X-ray Absorption Spectroscopy (XAS). Co-doping tunes the morphology of $V_2O_5$ nanostructure. Thus, the analytical results reveal that the co-doped $V_2O_5$ is a potential candidate with improved optical properties and electrochromic performance in comparison with $V_2O_5$.

**j0070**
**$V_2CT_x$/PPy Nanotube Hybrid Electrodes: Toward Superior Energy Storage in Asymmetric Supercapacitors**
Swarnalata Maity[a)] and Shyamal Kumar Saha[a,c]
[a]*School of Materials Sciences, Indian Association for the Cultivation of Science, 2A and 2B Raja S. C. Mullick Road, Jadavpur, Kolkata, 700032, West Bengal, India*
[c]*Academy of Innovative Semiconductor and Sustainable Manufacturing, National ChengKung University, Tainan, 701, Taiwan, ROC*
[*]*Email: swarnalatamaitys@gmail.com*
To meet the growing demand for efficient and sustainable energy storage, a hybrid electrode material combining $V_2CT_x$ MXene and polypyrrole (PPy) nanotubes was developed via in-situ polymerization. This composite effectively mitigates MXene restacking, enhances conductivity, and improves structural stability. The optimized $V_2CT_x$/PPyNT electrode achieved a high specific capacitance of 658 F $g^{-1}$ at 1 A $g^{-1}$, significantly outperforming pristine PPy and bare MXene. An asymmetric supercapacitor assembled with $V_2CT_x$/PPyNT-50@rGO delivered excellent energy and power densities, along with greater than 80% retention over 10,000 cycles, highlighting its promise for next-generation supercapacitor applications.

**j0071**
**First-Principles Investigation of Rhodium-Functionalized Cyclo[2n]carbons (n = 3–9) for $CO_2$ Sensing**
Ashvin Kanzariya*[,1], Shardul Vadalkar[2], L.K. Saini[1], Prafulla K. Jha[3]
[1]*Department of Physics, Sardar Vallabhbhai National Institute of Technology, Surat, Gujarat, India – 395007*
[2]*Department of Applied Science & Humanities, Sardar Vallabhbhai Patel Institute of Technology, Vasad, Gujarat, India – 388306*
[3]*Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, India – 390002*
[*]*E-mail: kanzariyaashvinbhai@gmail.com*
In this study, first-principles DFT calculations were conducted to investigate the $CO_2$ sensing performance of Rh-functionalized cyclo[2n]carbons (n = 3–9), a series of sp-hybridized carbon nanorings with tunable electronic properties. Although cyclo[8]carbon remains unsynthesized, its negative cohesive energy and absence of imaginary vibrational frequencies indicate thermodynamic stability and synthetic feasibility. $CO_2$ adsorption energies range from –0.52 to –0.58 eV, suggesting moderate physisorption favorable for reversible sensing, with adsorption distances between 2.28 and 2.31 Å. Upon $CO_2$ adsorption, notable changes were observed in the HOMO–LUMO gap and Fermi level, particularly for Rh@$C_8$ ($\Delta E_G$ = 30.42%, $\Delta E_F$ = 32.22%) and Rh@$C_{10}$ ($\Delta E_F$ = 41.81%), indicating strong electronic sensitivity. Work function values (4.20–4.88 eV) confirm charge redistribution at the sensor interface. Recovery time decreases significantly with ring size, from 4787.07 µs (Rh@$C_8$) to 519.38 µs (Rh@$C_{16}$), highlighting enhanced desorption kinetics in larger rings. Rh@$C_8$ exhibited the highest sensing response (354.17), while Rh@$C_{12}$, Rh@$C_{14}$, and Rh@$C_{16}$ offered a balanced combination of adsorption strength, recovery time, and signal transduction. These results underscore the potential of Rh-decorated cyclocarbons as efficient, tunable $CO_2$ sensing materials.

**j0072**
**High Active Material Loading $V_2O_5$ Electrodes with PVDF Binder for Superior Supercapacitor Performance**
Prakash Ganapati Anvekar[1,2], Ramachandra Naik[1]*, Nagaswarupa H.P[3]
[1]*Department of Physics, New Horizon College of Engineering, Bengaluru, VTU Belagavi - 560103, India.*
[2]*Department of Physics, Government Arts and Science College (Autonomous), Karwar - 581301, India.*
[3]*Department of Studies in Chemistry, Shivagangothri, Davangere University, Davangere - 577007, India.*
*Corresponding Author- Ramachandra Naik, *Email: rcnaikphysics@gmail.com, 7204408041*
The Vanadium pentoxide ($V_2O_5$) nanomaterial was successfully synthesized via the solution combustion method. Structural and morphological characteristics were thoroughly investigated using X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). The elemental composition of the synthesized $V_2O_5$ was confirmed through X-ray photoelectron spectroscopy (XPS). An electrode was fabricated by directly coating the $V_2O_5$ nanomaterial onto a nickel foam substrate. The electrochemical performance of the electrode was evaluated using cyclic voltammetry (CV), electrochemical

impedance spectroscopy (EIS), and galvanostatic charge–discharge (GCD) techniques. The fabricated electrode exhibited a specific capacitance of 147 F/g, Rct of 3.12 Ω and nearly symmetric charge discharge curves demonstrating its potential as a promising material for high-performance supercapacitor applications.

**j0074**

**Interconnected Porous Substrate Decorated with Silver Nanostructures for Efficient Clean Water Production**

Taniya Rabha[1], Anitha Thomas[2], Mohit Kalera[1] and Satish Laxman Shinde[1,a)]
[1]*Department of Physics, Indian Institute of Technology Hyderabad, Kandi, 502285, Telangana, India*
[2] *Center for Interdisciplinary Programs, Indian Institute of Technology Hyderabad, Kandi, 502285, Telangana, India*
**email: shindesl@phy.iith.ac.in*

Interfacial steam generation is proved to be one of the most effective methods for solar water purification. Here, we propose to enhance water evaporation efficiency by converting sunlight into heat using silver particles of different shapes. The silver nanostructures were coated onto commercially available, low-cost melamine sponge. The uniform and interconnected porous structure of sponge support the silver coating and improves water transport. Under 1 Sun illumination, the silver-decorated sponge showed high evaporation efficiency of ~84% and ~93% for silver nanoparticles (NPs) and nanocubes (NCs), respectively. The structural effect of sponge, strong LSPR, and extrinsic size effect of Ag NCs are majorly contributing for the efficient performance of NCs over NPs. Studying the influence of particle shape shows potential for further improving efficiency for the electromagnetic confinement and heat generation. This approach can show strong potential for finding cost-effective materials for practical applications in solar-driven water purification and desalination systems.

**j0075**

**Crystal Structure and Stability of Aluminum-Ion Battery Materials: A Density Functional Theory Study**

Sheetal Sisodiya[1,a)], Munendra Jain[1]and Ajay Phirke[2]
[1]*School of Technology Management & Engineering, SVKM`s NMIMS, Indore-453112*
[2]*Mukesh Patel School of Technology Management & Engineering, Mumbai-400056*
[a)]*Corresponding author: sheetal.sisodiya75@gmail.com*

Aluminum-ion batteries (AIBs) have emerged as a viable alternative to lithium-ion systems due to aluminum's high charge density, low cost, and natural abundance. The performance and stability of AIBs are fundamentally governed by the crystallographic structure of the active materials. In this study, we employ Density Functional Theory (DFT) to investigate the crystal structures, phase stability, and ion intercalation behavior of candidate electrode materials for AIBs, including aluminum-based intercalation compounds, metal oxides, and carbon-based hosts. Structural parameters such as lattice constants, bond lengths, formation energies, and electronic properties were computed and analyzed. The interaction of aluminum ions ($Al^{3+}$ and complex ions like $AlCl_4^-$) with host crystal lattices was studied to understand their diffusion pathways and lattice distortion upon intercalation. The results provide a comprehensive understanding of the structural dynamics that influence the electrochemical performance of AIBs and identify stable crystal phases with promising properties for future battery designs.

**j0076**

**Electrochemical Insights of Vanadium Hexacyanoferrate Thin Films for Supercapattery Applications**

Nilasha Maiti[1, 2,*], Pramod Bhatt[1, 2], Sher Singh Meena[1]
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400 085, India*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai 400 094, India*
**Email: nilasham@barc.gov.in*

The vanadium hexacyanoferrate (VHCF) thin film was electrochemically synthesized and evaluated as a cathode material for energy storage devices, including batteries and supercapacitors. It was deposited on a glassy carbon electrode via cyclic voltammetry by sweeping the potential from 0 to 1.2 V in an electrolyte solution containing $Na_3VO_4$, $K_3[Fe(III)(CN)_6]$ and $H_2SO_4$ compounds. A distinct pair of redox peaks was observed, attributed to the redox activity of hexacyanoferrate species in the electrolyte. The VHCF thin film exhibited a high specific capacity of 79 mAh/g and a specific capacitance of 260 F/g at a current density of 1.5 A/g. In addition to operating efficiently within a wide voltage window of 0–1.2 V, the film demonstrated excellent cycling stability over 500 cycles at varying current densities.

**j0077**

**Synthesis of $LuH_3$ using Sievert Method**

Ajay K. Mishra[1,3], Nishant N. Patel[1], Ajinkya P. Khangal[1,3] and Seemita Banerjee[2,3]
[1]*High Pressure & Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Mumbai-400085*
[2]*Chemistry Division, Bhabha Atomic Research Centre, Mumbai-400085*
[3]*Homi Bhabha National Institute Anushaktinagar, Mumbai-400094*
**Email:akmishra@barc.gov.in (Email of corresponding author)*

Hydrides are potential materials from superconductivity point of view as well as important for energy storage. Here, in this manuscript we have used Sievert apparatus to synthesize higher hydride of lutetium (Lu). In the present method hydriding of lutetium was carried out at 160°C and at 5 bar pressure using Au coated copper reactor of Sievert's type set up. Lu reaches its saturation value within 2 mins. The kinetics of hydrogen absorption further enhances with increasing the temperature from 160°C

to 250°C. Thus synthesized lutetium hydride is characterized using synchrotron based angle dispersive X-ray diffraction technique. The hydrogen stoichiometry is constrained based on the volume comparison of pure element and synthesized hydride compound. It turns out that the synthesized hydride is $LuH_3$ where volume expansion per hydrogen atom is ~ 1.8 $Å^3$. The lattice parameter of $LuH_3$ is determined to be $\boldsymbol{a} = \boldsymbol{b}$ = 6.177 (2) Å and $\boldsymbol{c}$ = 6.4350 (3) Å. Raman spectroscopic measurement of this compound reveal twelve number of Raman modes observed for this compound.

**j0078**

**Impact of Neodymium Oxide on the Local Structure and Connectivity of Tellurite Glasses**

Sourabh Wajhal[1,2,a], S K Mishra[1,2], A B Shinde[1] and P S R Krishna[1]
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai – 400085*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai – 400094*
**Email:swajhal@barc.gov.in*

The structure of Neodymium-Tellurite glass systems has been investigated using total neutron diffraction, complemented by Reverse Monte Carlo modelling. Three-dimensional atomic configurations were generated to analyse the glass network and evaluate short-range structural correlations. The coordination number distributions were determined for varying concentrations of Nd2O3. Notably, an increase in the average Te coordination number was observed with higher Nd2O3 content—an outcome that contrasts with previously reported trends in the literature. These results provide new insight into the role of rare earth modifiers in tellurite glass structures

**j0079**

**Structural and Optical studies of Sn doped $In_2Te_3$ Crystals**

Divyesh Patel[1], Ketan Chaudhari[1, a)], P H Soni[1]
[1]*Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara-390002, India*
**Email: k.h.chaudhari-phy@msubaroda.ac.in*

This research investigates the impact of Tin (Sn) doping on the structural and optical properties of Indium Telluride (In2Te3) crystals. In2Te3 crystals with varying Sn concentrations were successfully grown using the Bridgeman Stockbarger melt growth method. The powder XRD of (In2-XSnXTe3, X=0.00, 0.05), crystals were obtained & analyzed. The FTIR in the range between 400 cm-1 to 5500cm-1 wave numbers were obtained and analyzed.

**j0080**

**Enhanced Supercapacitor Performance Using 1T/2H Phase $MoS_2$/Functionalized MWCNT Composite**

Virendra Singh Choudhary[1] and Surender Kumar Sharma[1, a]
[1]*Department of Physics, Central University of Punjab, Bathinda, India - 151401*
[a)]Corresponding author: surender.sharma@cup.edu.in

A composite of 1T/2H phase molybdenum disulfide ($MoS_2$) and functionalized multi-walled carbon nanotubes (f-MWCNTs) was successfully synthesized and evaluated for supercapacitor applications. Structural analysis using XRD confirmed phase coexistence, while FESEM revealed a uniform distribution of $MoS_2$ nanosheets over the carbon network. Electrochemical characterization in 6 M KOH demonstrated a specific capacitance of **349.84 F/g**, an energy density of **50.2 Wh/kg**, and a peak power density of **6000 W/kg**, with low internal resistance (**Rb = 1.2 Ω, Rct = 3.26 Ω**). These results suggest the composite as a promising electrode material for next-generation energy storage systems.

**j0081**

**Controlled Growth of Cu-Based Quaternary Semiconductors via Hydrothermal Route: Role of Capping Agents**

Sonali M. Pingale[1,2], Sandesh R. Jadkar [1,*] Rohidas B. Kale[2,*]
*1. Photovoltaic lab, Department of Physics, Savitribai Phule Pune University, Pune – 411007 (India)*
*2. Department of Physics, The Institute of Science, Madam Cama Road, Mumbai – 400032 (India)*
*Email: rb.kale.phy@gmail.com*

For over a decade, copper-based quaternary chalcogenide semiconductors have been appealing materials in a variety of ways. The characteristics of capping agent variation in the copper-based quaternary chalcogenide $Cu_2NiSnS_4$ (CNTS) are clarified in this article. Here, we have hydrothermally synthesised CNTS in a range of capping agents, including 1 g, 50 mg, and 100 mg without Polyvinylpyrrolidone (PVP), at 180°C for 24 hours. Several techniques were used to characterise the properties of the prepared material, including phase purity, and powder X-ray diffraction analysis (XRD) was used to confirm the structure. Morphology is examined via the scanning electron microscope (SEM). With a band gap of around 1.57 to 2.5 eV, UV–vis spectrophotometry suggests a possible use in inexpensive thin-film solar cells. The prepared CNTS materials have a possible application in the optoelectronic and photovoltaic fields due to the observed properties

Keywords: Quaternary semiconductors, constant temp, Capping agent variation.

**j0082**

**Synthesis of Pd Thin Films by Electroless Metallization and Their Application in $H_2$ Sensing**

Niyanta Datta[1, a)] Deepa Bhambure[1], Kailasa Ganapati[1], Soumen Samanta[1], Manmeet Kaur[1,2]
[1]*Technical Physics, Division, Bhabha Atomic Research Center, Mumbai- 400085*

[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai- 400094.*
**Email: niyanta@barc.gov.in*
Hydrogen ($H_2$) is emerging as a clean, high-energy-density alternative to fossil fuels, but its high flammability demands fast and reliable leak detection. In this study, palladium (Pd) thin films were synthesized via electroless metallization—a simple, cost-effective, and scalable technique—on Pt-100 RTDs for $H_2$ sensing applications. The process employed $PdCl_2$ as the metal precursor and hydrazine-based reduction under mild conditions (50–80 °C), with $Sn^{2+}/Pd^{2+}$ sensitization to promote uniform nucleation. X-ray diffraction confirmed the face-centered cubic (fcc) structure of Pd with characteristic broadening from thin film geometry. Kelvin probe mapping revealed a uniform work function of ~4.7 eV with <1% variation. Integrated into a temperature-controlled Wheatstone bridge circuit, the Pd-coated RTD exhibited a linear voltage response to $H_2$ concentrations up to the lower explosive limit (4%), reaching 1.7 V at LEL. These results demonstrate the potential of electrolessly deposited Pd films for low-cost, scalable hydrogen sensing.

**j0083**
**Material Synthesis and Characterization of NbFeSb and $NbFeSb_{0.85}Sn_{0.15}$ Thermoelectric Material**
Ranu Bhatt[1,2,*], Angad Singh[1,3], Niyanta Datta[1], Pankaj Patro[2,4], Shovit Bhattacharya[1,2], Ajay Singh[1,2]
[1]*Technical Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, India*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai-400094, India*
[3]*Indian Institute of Science Education and Research, Pune-411008, India*
[4] *Powder Metallurgy Division, Bhabha Atomic Research Centre, Vashi Complex, Navi Mumbai-400703, India*
**Email: rbhatt@barc.gov.in*
Half Heusler are promising thermoelectric material for the mid-temperature range application due to their good mechanical stability, and moderate *zT*. In present paper we have investigated the thermoelectric response of NbFeSb and $NbFeSb_{0.85}Sn_{0.15}$ under inclusion of ball-milling step after arc-melting. Interestingly, inclusion of milling resulted in the formation of a metastable amorphous microstructure along with the crystalline peaks corresponding to NbFeSb and $FeSb_3$ phases. Intermediate milling has shown significant improvement in the power factor value of the material, showing a maximum power factor value of 150 μW/m-$K^2$ and 308 μW/m-$K^2$ for NbFeSb and $NbFeSb_{0.85}Sn_{0.15}$, respectively. The results are explained in term of Sb loss and formation of antisite defects.

**j0084**
**$Ln_3U_{11}O_{36}$ (Ln=La, Nd, Sm, Gd); A New Meta-Stable Phase Observed in U-Ln-O System.**
Muhammed Shafeeq, Geeta Patkare and Rohan Phatak
*Fuel Chemistry Division, Bhabha Atomic Research Centre, Mumbai-400085, Maharashtra, India.*
**Email: raphatak@barc.gov.in*
A new metastable phase with composition $Ln_3U_{11}O_{36}$ with mixed oxidation state of uranium was observed in the U-Ln-O system. The XRD pattern of the new phase is similar to $U_3O_8$ with some additional super lattice reflections. The detailed analysis shows that this phase is isostructural with the $Pb_3U_{11}O_{36}$ / $Sr_3U_{11}O_{36}$ structure. Various +3 cations were added to the Ln site in $Ln_3U_{11}O_{36}$ to check the effect of ionic radii. Feasibility of forming new phase decreases with decrease in ionic radii. Thermal stability study of $Ln_3U_{11}O_{36}$ phase shows this phase is stable up to 1223K in air.

**j0085**
**Exploring the Electrochemical Performance of $SrMoO_4$**
C. Muthuchamy[1], I. Ajin[1], T. Lavaneethan[1], and A. Chandra Bose[1,*].
[1]*Nanomaterials Laboratory, Department of Physics, National Institute of Technology, Tiruchirappalli 620 015, India*
**Email:acbose@nitt.edu*
The scheelite structured $SrMoO_4$ is synthesized via co-precipitation method. Through the XRD analysis the crystal structure and lattice parameters have been analyzed. The electrochemical studies reveal that the sample, calcinated at 800 °C, coated on nickel foam shows high specific capacity of 344 C $g^{-1}$ at the specific current of 1 A $g^{-1}$. It holds the Coulombic efficiency of 99.5 % at the specific current of 10 A $g^{-1}$ after 10000 charge-discharge cycles, which exhibits the good stability of the electrode material.

**j0087**
**Electrolyte Optimization for MXene-Based High-Performance Supercapacitors**
Shubham Mural[1], Shweta Tanwar[1], Anurag Gaur[1]*
[1]*Department of Physics, Netaji Subhas University of Technology, New Delhi- 110078, India*
**Email: anuragdph@gmail.com*
This work explores the impact of the different nature of electrolytes on the specific capacitance of MXene-based supercapacitors through various electrochemical analyses. Analysis performed using a basic electrolyte (1M KOH) and a neutral electrolyte (1M $Na_2SO_4$). The MXene electrode-based supercapacitors displayed a highest specific capacitance ($C_s$) of 146.33 F $g^{-1}$ (@ 10 mV $s^{-1}$) in 1M KOH. Remarkably, a significant enhancement was observed in 1M $Na_2SO_4$, where it reached 749.25 F $g^{-1}$ at the same scan rate. These findings underscore the significance of electrolytes in enhancing the charge storage capability of MXene electrodes, offering guidance for the development of high-capacitance supercapacitors in energy storage applications.

**j0090**

**Theoretical Insight Into The Excitonic Effects In The PtSSe Janus Layer**

Fidha Saheer M[1,2] Anjana E Sudheer[2] G. Tejaswini[2], Karthikeyan C[2], Muthu Vallinayagam[3] Mathias zschornak[3], Mathias posselt[4] and D Murali[2a)]

[1]*Department of Physics, Aligarh Muslim University,Uttar Pradesh,202002,India*

[2]*Department of Sciences, Indian Institute of Information Technology Design and Manufacturing, Kurnool, India.*

[3]*IEP,TU Bergakademie Freiberg, 09599 Freiberg, Germany, Fakultat Maschinenbau/Energietechnik/Physik, Hochschule fur Technik und Wirtschaft 01069 Dresden, Germany*

[4]*Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany*

*dmurali@iiitk.ac.in*

The two dimensional transition metal dichalcogenide Janus layers exhibit strong light-matter interaction and intense dielectric spectra. Here, we present structural, electronic and optical properties of the PtSSe Janus layer explored using first principle based Density Functional Theory (DFT) based calculations. To incorporate quasi particle interactions in the calculation, we depend many body perturbation theory based GW formalism. In addition, the excitonic effects are studied by solving the Bethe Salpeter Equation. The excitonic binding energy is optimized by varying the different parameters in the GW-BSE calculations. The presence of bound excitons in the designed JL is identified from the GW-BSE dielectric spectra. Further, the bright and dark excitons were identified from the oscillation strength of the excitons. The fat band analysis helped to analyse the spatial distribution of excitons are in the high symmetry point Γ-K-M. We also explore the excitonic wavefunction in the real space.

**j0092**

**Enhanced Specific capacitance in Ni-doped $Mn_2O_3$ Nanoparticles**

Keshav Kumar, Deepankar Das, Sahil, Chandana Rath*

*School of Materials Science and Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi-221005, India*

** crath.mst@iitbhu.ac.in*

In this work, we report the effects of Ni doping on structural and electrochemical properties of $Mn_2O_3$ nanoparticles prepared by sol-gel method. X-ray diffraction pattern demonstrates the cubic structure with space group Ia-3. The cyclic voltammetry (CV) results confirm that the $Mn_{1.90}Ni_{0.10}O_3$ electrode shows the maximum specific capacitance 454 F/g, in 2M KOH at 10 mV/s scan rate. This research demonstrates that the incorporation of Ni in $Mn_2O_3$ improves the conductivity of the nanomaterial and enhances the pseudo-capacitance.

**j0093**

**Enhanced Crystallinity Leading to Superior Photocatalytic Hydrogen Yield in g-$C_3N_4$**

R. V. Singh[1, 2], A. M. Banerjee[1, 2], S. Nath[2,3] and M. R. Pai[1, 2, a)]

[1]*Chemistry Division, Bhabha Atomic Research Centre, Mumbai – 400085, India*

[2]*Homi Bhabha National Institute, Training School Complex, Anushaktinagar, Mumbai 400085, India*

[3]*Radiation & Photochemistry Division, Bhabha Atomic Research Centre, Mumbai – 400085, India*

[a)]*Corresponding author: Email: mrinalr@barc.gov.in; mrinalpai9@gmail.com*

Photocatalytic water splitting using solar energy is a sustainable and promising approach for hydrogen ($H_2$) production. Among various photocatalysts, graphitic carbon nitride (g-$C_3N_4$) has attracted attention due to its visible light absorption and metal-free nature. However, traditional synthesis methods often yield amorphous g-$C_3N_4$ with limited photocatalytic efficiency, primarily due to rapid charge carrier recombination. Current study focuses on enhancing the photocatalytic performance of g-$C_3N_4$ by improving its crystallinity. Crystalline g-$C_3N_4$ (Cry-CN) samples were synthesized via thermal polymerization of melamine in vacuum-sealed quartz tubes. The synthesized catalysts were characterized using a range of techniques viz. XRD, UV-Vis DRS, PL, femtosecond transient absorption spectroscopy (fs-TAS), and electron microscopy. Fs-TAS revealed prolonged charge carrier lifetimes and reduced electron trapping in Cry-CN, attributed to its improved crystallinity and more efficient charge separation. Cry-CN exhibited enhanced photocatalytic $H_2$ evolution @70.8 µmol/h/g, which further increased to 108.4 µmol/h/g upon dispersion of Pt-cocatalyst compared to negligible from its amorphous counterpart.

**j0094**

**Reinforcement of Magnetic Filler in Polyaniline for X-band EMI Shields**

Ruchika Sharma[1] and Dwijendra P. Singh[1, a)]

[1]*Department of Physics and Materials Science, Thapar Institute of Engineering and Technology, Patiala, Punjab (147001).*

[a)] *Corresponding author: dpsingh@thapar.edu*

Polyaniline nanocomposites have gained so much of attention in the field of electromagnetic interference shielding due to conducting behavior of polyaniline. The present work aims at introducing LSMO (Lanthanum Strontium Manganite) in polymer matrix during *in-situ* chemical oxidative polymerization technique. The hybrid nanocomposite has been prepared in the ratio of 1:0.5, and 1:1 of polyaniline and LSMO named as P1L0.5, and P1L1 respectively. The conductivity of polyaniline increases with increasing LSMO content due to its colossal magneto resistive behavior. The highest value of conductivity has been achieved by P1L1 = 0.2 S/cm. The electromagnetic shielding study has been performed using vector network analyzer. The nanocomposite achieving highest value is P1L1 having SE ~28.5 dB. Shielding effectiveness is dominated by absorption with value ~20.5 dB

while reflection appears to be ~8 dB. The achieved value of shielding effectiveness makes this material to be used as shield for communication purposes.

**j0096**

**Stability Analysis of Phosphate Glass on Loading With Simulated Nuclear Waste**

Akhilesh C. Joshi[1, a)], Dimple P. Dutta[2] and S. N. Achary[1]
*[1]Chemistry Division, Bhabha Atomic Research Centre, Mumbai 400085, INDIA [22]Human Resource Development Division, Bhabha Atomic Research Centre, Mumbai 400085, INDIA*
*[a)] Corresponding author: acjoshi10@gmail.com/acjoshi@barc.gov.in*

One of the Generation IV (Gen IV) reactors are the molten salt reactors (MSR) which uses alkali metal fluorides both as fuel and coolant. Iron phosphate glass (IPG) was explored as an immobilization matrix for vitrification of simulated high-level nuclear waste generated from MSR. In this study, fluorides of Na, Ca, Nd, Ce and Sm were loaded inside iron phosphate glass to obtain their threshold concentration which forms a homogeneous glass. Stability of the formed glasses were studied using XRD, TG/DTA, etc. The thermal stability of IPG has been assessed using thermogravimetric-differential thermal (TG/DTA) analysis by calculating the glass stability (GS) and glass forming ability (GFA) parameters. TG/DTA analysis showed the high thermal stability and glass forming ability of the simulated nuclear waste loaded glass. XRD and SEM/EDX inferred the limiting concentration of the loaded elements which leads to the formation of homogeneous glassy phase. This study suggests the viability of IPG for immobilization of nuclear waste containing radioactive metal fluorides.

**j0097**

**Temperature Dependent Synthesis of $CsPbBr_3$ Perovskite and Its Enhanced Electrocatalytic Performance for Hydrogen Evolution Reaction in Alkaline Medium**

Surajit Tudu[2,1,a)] and Dipankar Chattopadhyay[1,2,b)]
*[1]Department of Polymer Science and Technology, University of Calcutta, Kolkata-700009, West Bengal, India.*
*[2]Centre for Research in Nanoscience and Nanotechnology, University of Calcutta, Kolkata-700106, West Bengal, India.*
*[b)]Corresponding author: dcpst@caluniv.ac.in*

This work explores the synthesis of Cesium lead bromide ($CsPbBr_3$) perovskite at varying temperatures and investigates its performance as an electrocatalyst for hydrogen production through electrochemical water splitting. $CsPbBr_3$ perovskite till now has not been explored more. The greatest challenge of one catalyst is to show both hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). In this study $CsPbBr_3$ has been studied for both but it shows better result at one of the varying temperature showing overpotential of 135 mV against 10 mA $cm^{-2}$ and 570 mV against 50 mA $cm^{-2}$ for HER.

**j0100**

**Structural, Electronic and Photocatalytic properties of $WS_2$/bg-$C_3N_4$ Hetero-Structure: A DFT study**

Saurabh Bhatia[1, (a)], Anjali[1], Shivani Sharma[1], Bharti Thakur[1], Yogyata Pathania[2], Surjeet Kumar Chandel[1] and Arun Kumar[1]
*[1]Govt College Bilaspur, 7, Bilaspur, Kosrian Sector, Bilaspur, Upmohal Oel, Himachal Pradesh 174001*
*[2]Department of Physics, DAV Post Graduate College Sector 10, Chandigarh 160011*
**Email: saurabh.btia19@gmail.com*

This work explores the potential of the $WS_2$/bg-$C_3N_4$ heterostructure as an efficient photocatalyst for hydrogen evolution. Using DFT calculations, the structural and electronic properties of the heterostructure were studied. The results show a notable modification in the electronic structure, including reduced band gap and improved charge separation due to the formation of the heterojunction. These enhancements ultimately contribute to the photocatalytic activity by promoting more efficient electron transfer across the interface. Overall, the results highlight $WS_2$/bg-$C_3N_4$ heterostructure as a strong candidate for sustainable hydrogen evolution in acidic medium via photocatalytic water splitting.

**j0101**

**Study of Optical and Electrochemical Properties of $Mg_{0.7}Co_{0.3}Fe_2O_4$ Nanoparticles**

Malavika A. S.[1], Abdul Nafih A. A.[1], Dana S. Abraham[2], Anna Rose Binu[1], M. Bhagiyalakshmi[2], Subasa C. Sahoo[1,*]
*[1]Department of Physics, Central University of Kerala, Tejaswini Hills, Periya, Kasaragod, Kerala 671325 India*
*[2]Department of Chemistry, Central University of Kerala, Tejaswini Hills, Periya, Kasaragod, Kerala 671325, India*
**Email:subasa.cs@gmail.com*

$Mg_{0.7}Co_{0.3}Fe_2O_4$ nanoparticles were synthesized using the co-precipitation method and were annealed at 900°C. X-ray Diffraction (XRD) studies confirmed the formation of single-phase spinel structure in the sample with crystallite size of 21.7 nm. UV-Vis spectroscopy revealed a direct bang gap of 1.86 eV. Electrochemical properties evaluated through cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS) demonstrated promising supercapacitor behavior. The quasi-rectangular CV curves indicated reversible and stable redox activity, while GCD measurements yielded a maximum specific capacitance of 23.4 F $g^{-1}$ at a current density of 0.5 A $g^{-1}$. The specific capacitance decreased with the increase in current density. The EIS Nyquist plot exhibited a semicircular profile, characteristic of charge-transfer resistance.

**j0102**

**Computational Investigation of CO2 Electroreduction on Palladium-Functionalized Two-Dimensional Polyaramid: A First-Principles Study**

A T Sathya [1,*], Ravi K Trivedi [2,3], Kunal Shaw [1] and Brahmananda Chakraborty [4,5]
[1]*Department of Physics, Indian Institute of Technology Roorkee, Roorkee 247667, Uttarakhand, India*
[2]*Department of Physics, Karpagam Academy of Higher Education, Coimbatore 641021, Tamil Nadu, India*
[3]*Centre for Computational Physics, Karpagam Academy of Higher Education, Coimbatore 641021, Tamil Nadu, India*
[4]*High Pressure and Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai, India-400088*
[5]*Homi Bhabha National Institute, Mumbai, India-400088*
**Email: a_tsathya@ph.iitr.ac.in*

This work presents a comprehensive first-principles investigation into the catalytic performance of palladium-decorated two-dimensional polyaramid (2DPA) for electrochemical carbon dioxide reduction reaction (CO2RR). Our density functional theory calculations reveal Pd binding to the 2DPA substrate with an adsorption energy of -0.62 eV, facilitated by substantial electron redistribution from Pd 4d states to the aromatic π-network of the host material. Electronic property analysis demonstrates that Pd functionalization converts the initially semiconducting 2DPA into a conducting material, significantly boosting its electrocatalytic potential. Thermal stability assessment through ab initio molecular dynamics at 300 K confirms structural robustness with negligible atomic displacement fluctuations. The adsorption energies of the reaction intermediates for CO2 reduction reactions had been investigated. The reaction free diagram to produce those intermediates awaits continued investigation. This study highlights the promising potential of Pd functionalized 2DPA as an efficient and durable catalyst for CO2 reduction, contributing to the development of sustainable and effective CO2RR technologies.

**j0104**

**Trimetallic $MnCoFeO_4$ Nanostructure as Advanced Electrode Materials for Pseudocapacitive Energy Storage**

Saheli Ghosh[1], Ashik Ikbal[1], Arijit Ghosal[1], and Ruma Ray[1,*]
[1]*Department of Physics, Jadavpur University, 188 Raja S C Mallick Road, Jadavpur, Kolkata 700032, West Bengal, India*
[*]*Email: juphyruma@gmail.com (Email of corresponding author)*

The increasing demand for sustainable energy storage has shifted the focus to the fulfillment of efficient electrode active materials with high redox activity and conductivity. In this study, $MnCoFeO_4$ spinel ferrite nanoparticles were synthesized via the co-precipitation method and investigated as a pseudocapacitive cathode material. Structural characterization by XRD confirmed the successful formation of the $MnCoFeO_4$ spinel phase, while FESEM analysis showed uniformly distributed particles with an average size of ~26 nm. Electrochemical analysis using cyclic voltammetry (CV) and galvanostatic charge–discharge (GCD) in a three-electrode setup exhibited excellent specific capacitances of 663.42 F $g^{-1}$ at 2 mV/s and 765.3 F $g^{-1}$ at 1.5 A $g^{-1}$, respectively. The superior performance is attributed to the synergistic redox activity of Mn, Co, and Fe ions within the spinel lattice, which enables fast kinetics and efficient ion diffusion. These results highlight $MnCoFeO_4$ as a promising candidate for next-generation supercapacitor cathodes.

**j0105**

**Tailoring Electronic and Ionic Transport in Multimetal Sulfide Nanostructures with Precise $Ti_3C_2T_x$ MXene Incorporation for Supercapacitor Applications**

K. Lokeswara Rao* and Dr. D. Amaranatha Reddy
*Department of Sciences, Indian Institute of Information Technology Design and Manufacturing, Kurnool – 518007, India.*
**Email: 323ds0004@iiitk.ac.in*

The integration of multimetal sulfides with MXene in composite materials yields supercapacitors with exceptional electrochemical capabilities that surpass the performance of individual metal sulfides or MXenes. In this paper, we present the synthesis and evaluation of the electrochemical properties of a novel cobalt–nickel–molybdenum sulfide/MXene (CNMS-MXene) hybrid composite, specifically designed to enhance the performance of high-capacity supercapacitors. The CNMS nanorods are uniformly anchored onto exfoliated $Ti_3C_2$ MXene nanosheets via an ultrasonication-assisted self-assembly process, resulting in a well-defined hybrid architecture. Through this synergistic configuration, the composite exhibits remarkable electrochemical performance, achieving a specific capacity of 284.78 mAh/g at a current density of 1 A/g. Furthermore, it displays exceptional cycling stability, retaining 84% of its capacity after undergoing 10,000 charge-discharge cycles.
Keywords: Hydrothermal method, multimetal sulfides, high specific capacity, asymmetric supercapacitor.

**j0108**

**Enhancement of Charge Carrier Extraction in Carbon-Based Perovskite Solar Cells Utilizing $MAPbI_3$:NiO Nanoparticles**

R. Govindaraj[1, a)], R. Isaac Daniel[1], P. Ramasamy[1] and A. K. Chauhan[2]
[1] *Department of Physics, SSN Research Centre, Sri Sivasubramaniya Nadar College of Engineering, Kalavakkam-603110, Tamil Nadu, India*
[2] *Organic Devices Section, Technical Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400 085, India*
**Email:govindarajr@ssn.edu.in*

Various strategies employing perovskite composites combined with organic and inorganic materials have been developed to enhance the power conversion efficiency (PCE) of PSCs. In this study, we evaluated the performance of carbon-based Perovskite Solar Cells (C-PSC) using composites with p-type nickel oxide (NiO) semiconductor material at different weight percentages.

These results were compared to C-PSC made with pure methylammonium lead iodide ($MAPbI_3$) as the perovskite precursor. A single-step process was used to deposit the perovskite layers. The inclusion of P-type semiconductor material (NiO NPs) enhances the crystallinity of the perovskite film, leading to larger grain sizes and effective passivation of the perovskite grain boundaries, which reduces non-radiative recombination. The solar cell with 20 mg $mL^{-1}$ NiO NPs in the perovskite achieves a maximum PCE of 9.75%.

**j0109**

**Phase Segregation in $Ba_2FeVO_6$ Synthesis: Structural, Optical, and Photocatalytic Properties of $Ba_3V_2O_8$/$BaFeO_{2.654}$ Composite**

Shubha Dubey[1, a)], Gitanjali Pagare[2], and N. K. Gaur[1]
[1]*Department of Physics, Barkatullah University, Bhopal, 462 026, India.*
[2]*Departemnt of Physics, Sarojini Naidu Govt. Girls P. G. Autonomous College, Bhopal 462 016, India*
**Email: shubha.dubey4@gmail.com*

In this study, we report the synthesis and comprehensive characterization of a Ba–Fe–V–O composite aimed at realizing the $Ba_2FeVO_6$ double perovskite. Using a solid-state reaction method followed by calcination at 750 °C for 4 hours, two distinct crystalline phases—$Ba_3V_2O_8$ (R-3m) and $BaFeO_{2.654}$ ($P6_3/mmc$)—were obtained instead of a single-phase $Ba_2FeVO_6$. This phase segregation is attributed to thermodynamic instability, cation mismatch, oxygen non-stoichiometry, and limited diffusion during synthesis. Structural and spectroscopic investigations, including UV-Vis, PL, and XPS analyses, revealed critical insights into the local structure, optical response, and defect states within the multiphase composite. Photoluminescence and UV-Vis spectroscopy confirmed the presence of a narrow optical bandgap (~2.1 eV) and abundant defect states—particularly oxygen vacancies—which enhance visible-light absorption and suppress electron–hole recombination. Photocatalytic performance was evaluated via the degradation of Rhodamine B dye under visible-light irradiation, where the composite achieved over 90% degradation within 40 minutes. This superior activity is attributed to synergistic effects of phase coexistence, formation of a Type-II heterojunction, interfacial charge separation, and efficient generation of reactive oxygen species (ROS).

**j0110**

**Na-intercalation on graphene and $NbS_2$ heterostructure: A vdW dispersion corrected DFT Study**

B. Chettri[1], D.P Rai[1,a)]
[1]*Department of Physics, Mizoram University, Aizawl-796004, India*
[a)]*Corresponding author:dibyaprakashrai@gmail.com*

The graphene-$NbS_2$ heterostructure is explored as a sodium ion battery electrode using DFT calculations. Its stability is confirmed with a formation energy and AIMD calculation. Na adsorption energies lie from -3.04 to -1.57 eV with an OCV of 1 eV and a specific capacity of 403.89 mAhg-1, competitive to Cu2N and graphite. NEB calculations show diffusion barrier energy of 0.43 eV (cavity) and 0.15 eV(atop $NbS_2$) supporting efficient mobility. Further studies on the multiple layered stacked configuration are underway.

**j0111**

**Solvent-Induced Spectral Behavior of 7-Aminoflavone: Experimental and Computational Insights**

Sanjay Pant[1, a)], Nisha Fatma[1], Mohd Suhail[1], Pankaj Pant, Rakesh C. Joshi, and Nupur Pandey[1]
[1]*Department of Physics, DSB Campus, Kumaun University, Nainital, Uttarakhand*
**sanjayphotophys@gmail.com*

Excited state behavior of 7-Aminoflavone (7AF) has been explored through experimental (steady-state and time resolved) and computational approach. Large bathochromic shift in absorption and fluorescence spectra with solvent polarity was ascribed to intramolecular charge transfer (ICT) interaction. Calculations based on various solvent correlation techniques denote that the excited state dipole moment value is higher than the ground-state counterpart, hence indicates substantial redistribution of electron density in the excited state. Quantum chemical investigations were performed to evaluate various parameters such as dipole moments, energy of molecular orbitals, absorption and fluorescence wavelengths, electrostatic potential etc. which adequately reflect the experimental observations. Multiple linear regression (MLR) method reveals that photophysical behavior of 7AF is attributed to both specific and non-specific interactions. Changes observed in fluorescence lifetime parameters confirms the inclusion of ICT process. Practical applications of 7AQ have also been demonstrated indicating its future relevance in the realm of optoelectronics.

**j0112**

**Investigating the Synergistic Photocatalysis of $Bi_2Sn_2O_7$ and $C_3N_5$ Heterojunctions**

Adarsh Kumar[1,2*], Sagnik Mitra[1,2], Deepak Tyagi[1,2], Jitendra Bahadur[2,3], Avesh K. Tyagi[2], Kaustava Bhattacharyya[1,2*]
[1]*Chemistry Division, Bhabha Atomic Research Centre, Mumbai 400085, INDIA*
[2]*Homi Bhabha National Institute, Mumbai 400094, INDIA*
[3]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai -400 085, India*
**Email: adarshsinhachem@gmail.com*

In this study, we synthesized $Bi_2Sn_2O_7$-g-$C_3N_5$ (BSN-CN) heterojunctions to degrade ortho-dichlorobenzene (o-DCB), a surrogate for dioxins and furans. The close bandgap alignment between the materials enhanced charge separation. A detailed characterization

confirmed the heterojunctions and revealed how structural parameters influenced their photocatalytic performance under visible light. The BSN-CN composites exhibited superior activity compared to individual components. Notably, the BSN-CN-15 sample achieved the fastest and most complete mineralization of o-DCB reported to date. We established a clear structure-activity relationship, detailing how bandgap energy and surface charge govern efficiency. Post-reaction analysis also helped us understand the degradation mechanism and identify key intermediates, which can guide future catalyst design.

**j0113**

**Exploring Cerium Based Materials for Lithium Adsorption**

Deepak Tyagi[1,2*], Harshita Sharma[3], A. N. Shirsat[1,2], Salil Varma[1,2]
[1]*Chemistry Division, Bhabha Atomic Research Centre, Mumbai 400085, INDIA*
[2]*Homi Bhabha National Institute, Mumbai 400094, INDIA*
[3]*Jai Narain Vyas University, Jodhpur, Rajasthan 342011, INDIA*
**Email:dtyagi@gov.in*

Lithium extraction is essential due to the growing global demand for lithium-ion batteries, which are widely used in electric vehicles, portable electronics, and renewable energy storage systems. As conventional sources of lithium, such as hard rock mining and brine extraction, face environmental and economic challenges, alternative methods like adsorption from spent batteries are gaining attention for their efficiency and sustainability. In our study, various cerium-based adsorbents were evaluated for lithium adsorption, among which cerium hydroxide demonstrated the most promising performance. It achieved a lithium sorption capacity ranging from 13% to 23%, indicating its potential as an effective material for lithium recovery. This result highlights cerium hydroxide as a strong candidate for further development in advanced lithium extraction technologies.

**j0114**

**Structure and optical properties of 1D hybrid halide perovskite with morpholinium as spacer cation**

Dibya kanti Mal, [1] Sandeep Nigam[1 *)], C. Majumder[1]
[1]*Chemistry Division, Bhabha Atomic Research Centre, Mumbai,*
**snigam@barc.gov.in*

Low dimensional halide double perovskite ($A_2B^1B^2X_6$) has recently emerged as an alternative class of material for their promising performance in the field of optoelectronics. In this work, two hybrid organic inorganic perovskite (HOIP) materials with morpholinium as organic cation [$(Mor)_2KBiBr_6$ and $(Mor)_2KInCl_6$, Mor = Morpholinium] have been synthesized and characterized. The PXRD analysis indicates both systems to be crystallized into one dimensional monoclinic space group *C2/c*. The organic amine ligand not only maintaining charge balance but also coordinates to $K^+$ ion via $sp^3$ hybridized oxygen atom to stabilize the entire structure. The optical band gap for Bi based bromide HOIP was found to be less (e.g. ~3 eV) than corresponding In based chloride HOIP (~4.5 eV), indicating a profound influence of B site cation and halide ion on electronic structure of the system.

**j0115**

**Modification of polyvinyl alcohol film by addition of lignin nanoparticles for energy storage device applications**

Manali Pancholi[1], Debjani Bagchi[1,a)]
[1]*Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, India.*
*[a)]Corresponding author: debjani.bagchi-phy@msubaroda.ac.in*

Nowadays, the demand for utilizing biopolymer composites instead of using non-biodegradable synthetic polymers or other corrosive materials is increasing. To satisfy this purpose, fabricated composites of polyvinyl alcohol (PVA) induced with biopolymer nanoparticles, such as lignin nanoparticles (LNP), with various concentrations. LNP has been prepared using the Nanoprecipitation method and has a size of 149 ± 4 nm, as studied by the TEM image of LNP. The higher negative magnitude of zeta potential shows the excellent stability of LNP in water. The appearance of two peaks at 286 nm and 310 nm in the UV-vis spectra of PVA films with LNP shows the presence of LNP in PVA films. Using broadband dielectric spectroscopy, studied the dielectric properties of PVA films, either with or without LNP, across a frequency range of $10^{-2}$ Hz to $10^7$Hz. The fitted Nyquist plot shows that as the capacitance of the material and charge transfer resistance increase and decrease, respectively, with an increase in the concentration of LNP. Dielectric constant, dielectric loss, and tangent loss decreased with an increase in frequency. The dielectric constant increased 10 times by inducing LNP into PVA film at 0.01 Hz because the electrostatic interaction between LNP and PVA improved the dipole arrangement in PVA film. The decreasing order of dielectric tangent loss in the higher frequency region indicates that these composites can be applicable for energy storage devices in the higher frequency region without energy dissipation. Raising the concentration of LNP in PVA films led to an enhancement of AC conductivity and relaxation time, attributed to a reduction in the potential barrier for charge carriers and improved structural dynamics within the polymer matrix. The addition of LNP significantly improved the AC conductivity of PVA film from 4.8E-10 to 1.4E-9 S/m with rapid changes in the higher frequency region. The relaxation time decreased by 2.5 times compared to pure PVA film. Therefore, the enhancement of dielectric properties of PVA film by the addition of LNP can be applied in energy storage device applications to prepare devices that are lightweight, portable, and biocompatible.

**j0117**

**Pressure-driven Structural and Transport Modifications in $Li_xCoO_2$ with Layered and Rock-Salt Phase Coexistence**

A Jain[1,a], T. Maran[2], M. Sundaramoorthy[2,5], A. P. Roy [4], B. Joseph[5], G.Lingannan[2], A. Mohan [6], D. Bansal[4], S. M. Yusuf[1,3] , and A. Sonachalam [2,7]
*1Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400 085, India*
*2Center for High Pressure Research, Bharathidasan University, Tiruchirappalli - 620 024, India*
*3Homi Bhabha National Institute, Anushaktinagar, Mumbai 400 094, India*
*4Department of Mechanical Engineering, Indian Institute of Technology Bombay, Mumbai 400 076, India*
*5 Elettra - Sincrotrone Trieste S.C. p.A., S.S. 14, Km 163.5 in Area Science Park, Bosavizza 34149, Italy*
*6Department of Physics, Institute of Chemical Technology, Matunga, Mumbai 400019, India.*
*7Tamil Nadu Open University, Chennai- 600 015, India*
*[a] Email: ajain@barc.gov.in*
Voltage and capacity fading in Li-ion battery stem form lattice strain due to Li-ion insertion and extraction. We investigated $Li_xCoO_2$ single crystals (5% excess Li) and found a stable volume fraction of 60:40 of the rhombohedral and cubic phase up to 10.6 GPa. Transport and DFT studies show semi-metallic behavior enhanced by pressure, indicating high phase stability and potential as robust cathode material.

**j0118**
**Formation and Environmental Implications of Mercury–Water/Oxygen Cluster Complexes in the Gas Phase**
Vaibhav Chauhan,[1,a] Varun Vinayak Deshpande,[1,2] and Soumen Bhattacharyya[1,2]
*[1]Atomic & Molecular Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400 085, India.*
*[2]Homi Bhabha National Institute, Anushaktinagar, Mumbai 400 094, India.*
*[a]Corresponding author: vibhu9494@gmail.com*
We report the mass spectrometric identification of mercury–water/oxygen complexes formed via soft laser vaporization of aqueous mercury nitrite solution in the MALDI setup. The results reveal stable hydrated and oxidized Hg species, including $HgO_2(H_2O)n$ and nitrate-containing adducts. Such hydration–oxidation steps are crucial in atmospheric Hg transport, increasing solubility and deposition potential. These findings bridge laboratory observations with environmental processes, highlighting the role of hydrated Hg species in the atmospheric cycling, transport, and deposition of mercury into terrestrial and aquatic ecosystems.

**j0119**
**Enhancing Supercapacitive Capabilities of Ternary Metal Oxide Composite: Effect of Deposition Potential Pattern on Energy Storage**
Nikita Ahlawat, and Rajesh Kumar*
*Material and Devices Laboratory (MAD Lab) Department of Physics, Indian Institute of Technology Indore, India*
**Email: rajeshkumar@iiti.ac.in*
Tailoring electrode architecture through deposition strategy is a critical route toward enhancing the electrochemical performance of pseudocapacitive materials. Herein, we report the controlled fabrication of nickel cobaltite ($NiCo_2O_4$) manganese oxide ($MnO_2$) heterostructure complex (NCMO) electrodes via three distinct electrodeposition modes: constant electrodeposition (CED), pulse potential (PP), and pulse reverse potential (PRP) to elucidate their influence on morphology and energy storage properties. The CED mode yields a non-uniform film composed of large agglomerates, while PP produces a more homogeneous nano-flake structure. Remarkably, the PRP mode results in a fully interconnected flake–flower-like nanostructured network with significantly enhanced surface accessibility and electrical conductivity. The optimized PRP-deposited NCMO electrode delivers a high specific capacitance of 595.55 mF/cm$^2$, outperforming its CED (94.45 mF/cm$^2$) and PP (296.7 mF/cm$^2$) counterparts by factors of approximately 6 and 2, respectively. When integrated into an asymmetric supercapacitor device, the PRP-based electrode exhibits superior energy and power density, along with excellent cycling stability, retaining 83% of its initial capacitance over 1000 charge-discharge cycles. Furthermore, the device successfully powers a digital clock for approximately 4 minutes, underscoring its practical viability for low-power applications. These findings demonstrate that PRP electrodeposition is a robust and scalable strategy for engineering high-performance pseudocapacitor electrodes, offering significant promise for next-generation energy storage systems.

**j0120**
**Morphology-Controlled ZCS@PI Core-Shell Architectures for Enhanced Energy Storage in Asymmetric Supercapacitors**
Partha Sarathi Rout[1], Love Bansal[1], Rajesh Kumar*
*[1] Materials and Device Laboratory, Department of Physics, Indian Institute of Technology Indore, Simrol 453552, India*
**Email: rajeshkumar@iiti.ac.in*
Driven by the urgent need for sustainable energy storage, advanced supercapacitors with improved energy density were developed. Here, an asymmetric device featuring a core-shell zinc cobalt sulfide/polyindole (ZCS@PI) composite cathode paired with an activated carbon (AC) anode has been designed. Sequential double electrodeposition on nickel foam (NF) yielded a porous honeycomb ZCS core enveloped by polyindole nanosheets. Electrochemical testing revealed a superior specific capacitance of 4700 F g$^{-1}$ at 80 mA g$^{-1}$ for ZCS@PI, outperforming individual ZCS (2437 F g$^{-1}$) and PI (1690 F g$^{-1}$). The assembled ZCS@PI/AC device achieved a capacitance of 928 mF cm$^{-2}$ at 10 mA cm$^{-2}$, an energy density of 180.9 Wh cm$^{-2}$ at 1186.2 W cm$^{-2}$, and a maximum power density of 10.7 kW cm$^{-2}$ at 25.3 Wh cm$^{-2}$ . After 1000 cycles at 30 mA cm$^{-2}$, the device retained 102 % of its capacitance

and successfully powered LEDs and a DC motor. Combined EIS, in situ Raman, SEM, and simulations elucidated the roles of structure and redox interactions. This study advances scalable, robust core-shell supercapacitor design and deepens fundamental understanding of architecture-driven performance.

**j0121**

**Tuning The Thermoelectric Properties Of Multiwalled Carbon Nanotubes Sheets For Energy Harvesting**

Meetu Bharti*[1], Suman K. Mishra[2,3], Ajay Singh*[3,4]
[1]*All India Jat Heroes' Memorial College, Rohtak-124001, Haryana, India*
[2]*Advanced Tunable Laser Applications Division, Trombay, Mumbai-400085, India*
[3]*Homi Bhabha National Institute, Anushaktinagar, Mumbai, India*
[4]*Technical Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai-400085*
**Email: meetubharti@gmail.com*

Thermoelectric properties of free-standing carbon paper films synthesized from multi-walled carbon nanotubes (MWCNTs) were investigated. These free-standing paper films were treated with polymer polyethylenimine and interestingly, their conduction type showed transition from p- to n-type. The electrical conductivity of PEI-modified carbon paper enhances initially upto 5 wt% and after that, it lowers down to a great extent i.e. below the value obtained in case of pristine carbon paper samples. However, in order to enhance the thermoelectric performance of MWCNTs paper, dual doping with PEDOT:PSS and SnTe was carried out. The sequential energy dependent scattering of charge carriers at MWCNT and organic-inorganic interfaces caused significant improvement of Seebeck coefficient. The power factors values of ~ 0.2, ~0.4 and ~1.4 $\mu W/m/K^2$ were observed respectively for pure MWCNTs, MWCNT/PEDOT:PSS and MWCNT/PEDOT-PSS/SnTe nanocomposite sheets. The present work provides a facile technique to change conduction type along with improvement of thermoelectric properties of carbon paper films.

# k) 1-D, 2-D and quantum materials

**k0001**

**Microscopic Magnetic Correlations in Spin-1/2 Coupled-Dimer Compound $Cu_2P_2O_7$: A Neutron Diffraction Study**

B. Ghanta,[1,2] K. S. Chikara,[1,2] A. K. Bera[1,2 a)] and S. M. Yusuf[1,2]
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India;*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*
**Email: akbera@barc.gov.in*

We report the magnetic ground state and crystal structure of a spin-1/2 ($Cu^{2+}$) antiferromagnetic dimer compound $Cu_2P_2O_7$ by the temperature-dependent neutron diffraction study. Structural analysis reveals that edge-shared $CuO_5$ square pyramids form $Cu_2O_8$ structural dimers. Such dimers are coupled by $PO_4$ tetrahedra, leading to a complex interacting dimer system. Temperature dependent neutron diffraction patterns reveals the onset of long-range antiferromagnetic (AFM) ordering at $T_N$ ~25 K. All the magnetic Bragg peaks are indexed by a commensurate propagation vector $\boldsymbol{k}$ = (0, 0, 0). Magnetic symmetry analysis reveals an AFM structure with space group *C2*/*c*′. Our analyses yield an ordered magnetic moment of 0.66(8) $\mu_B$/$Cu^{2+}$ at 5 K. Critical exponent analyses determine the exponent $\beta$ = 0.369(3), consistent with a 3D Heisenberg universality class.

**k0002**

**Majorana Polarization in Disordered Heterostructures**

Shubhanshu Karoliya,[1,a)] Sumanta Tewari,[2] and Gargee Sharma[3]
[1]*School of Physical Sciences, Indian Institute of Technology Mandi, Mandi 175005, India.*
[2]*Department of Physics and Astronomy, Clemson University, Clemson, South Carolina 29634, USA*
[3]*Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi 110016, India*
[a)]*Email: ud22005@students.iitmandi.ac.in*

We investigate Majorana polarization as a diagnostic for identifying topological Majorana-bound states (MBSs) in Rashba spin-orbit coupled semiconductor systems with proximity-induced superconductivity and disorder. Focusing on both one-dimensional nanowires and quasi-one-dimensional systems, we show that while the condition $P^*_{left} \cdot P_{right} \sim -1$ can indicate Majorana signatures; it alone cannot reliably distinguish true topological MBSs from partially separated Andreev-bound states (psABS) or quasi-Majorana modes. Our results highlight that confirming topological MBSs requires, in addition to polarization, evidence of a topological gap and edge-localized wavefunctions. These conclusions hold for both chiral and particle-hole definitions of Majorana polarization, emphasizing the need for multifaceted diagnostics in disordered systems relevant to topological quantum computation (TQC).

**k0003**

**Effect of Co-catalyst and growth temperature during Graphene synthesis by PECVD method – analysed using Raman Spectroscopy**

Aditi Sonal[1,2], Harsha Kumawat[2,3], S.R. Vishwakarma[2], D. Dixit[1,4], P.T. Rao[5], J. Prakash[5,3], Himal Bhatt[2, a)]
[1]*Delhi Technological University, New Delhi 110042*
[2]*High Pressure & Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Mumbai 400085*
[3]*Homi Bhabha National Institute, Mumbai 400094*
[4]*Indian Institute of Science Education and Rsearch, Bhopal*
[5]*Glass & Amophous Materials Division, Bhabha Atomic Research Centre, Mumbai 400085*
**Email: hbhatt@barc.gov.in*

This study presents vibrational spectroscopic studies on graphene films synthesized by plasma enhanced chemical vapour deposition with cobalt catalyst. The grown films were characterized by Raman spectroscopy to assess the effects of catalyst sputtering time and growth temperature on structural quality, including defect density and estimation of number of layers. Optimal PECVD conditions were determined as 6 minutes of cobalt sputtering followed by growth at 800 °C to synthesize few-layer graphene with minimal defects

**k0004**

**Correlation Effects In Coupled Quantum Wires Using The Single Loop Random Phase Approximation**

Gautam Shah[1] , Vidit Gangwar[1] and Vinod Ashokan[1,*]
[1]*Computational Quantum Many-Body Physics Lab,*
*Department of Physics, Dr. B. R. Ambedkar National Institute of Technology, Jalandhar, Punjab-144008, India*
[*]*Email: ashokanv@nitj.ac.in*

The dynamical response theory is used to calculate the static structure factors, pair correlation functions, and correlation energies of an electron-electron quantum wires of confinement width *b* using the single loop random phase approximation. This study emphasis on how intra- and inter-wire correlations influences the structural properties. The intra-wire static structure factor and pair correlation function show minimal variation, whereas the inter-wire observables exhibit strong sensitivity to interwire separation *d*, with pronounced correlations emerging at small separations. Also, the correlation energy reveals a significant enhancement as *d* decreases, driven by strong inter-wire electron interactions. This behavior exhibits the enhanced role of inter-wire coupling *d*, highlighting the importance of spatial confinement in shaping many-body correlation effects in low-dimensional systems.

**k0005**

**Correlation Energies of the Quasi-One-Dimensional Ferromagnetic Electron Gas**

Vidit Gangwar[1], Gautam Shah[1] and Vinod Ashokan[1,*]
[1]*Computational Quantum Many-Body Physics Lab, Department of Physics,*
*Dr. B. R. Ambedkar National Institute of Technology, Jalandhar, Punjab - 144008, India*
**Email: ashokanv@nitj.ac.in*

We study the correlation energies of quasi-one-dimensional ferromagnetic electron gas for harmonic-delta confinement in the transverse directions. The singularity of the one-dimensional Coulomb potential at zero inter-particle distance is regularized by confining the motion of electrons in the transverse plane by a harmonic-delta potential. The first-order random phase approximation, including self and exchange-energy contributions, which provides ground-state structure beyond random phase approximation, is used to numerically compute the ground state properties, i.e. correlation and ground state energies. The correlation energy significantly depends on pragmatic widths $b$ and density parameters $r_s$. For the ultrathin wire in the high-density limit, the correlation energy converges to $-\pi^2/360$ a.u. for the harmonic-delta potential, in agreement with the exact results.

**k0006**

**Quantum Correlation Effects of 1D Trapped Electrons Confined in the Transverse Plane by Infinite Square-Well and a Triangular Potential**

Vinod Ashokan[1,*], Vidit Gangwar[1], and Gautam Shah[1]
[1]*Computational Quantum Many-Body Physics Lab, Department of Physics,*
*Dr. B. R. Ambedkar National Institute of Technology, Jalandhar, Punjab - 144008, India*
**Email: ashokanv@nitj.ac.in*

We study the ground-state properties (static structure factor, pair correlation function, ground state energy, and correlation energy) of quasi-one-dimensional electron gas. The electrons are confined in the *yz*-plane by transverse confinement of infinite square-well and a triangular potential. Within this framework we employ the first order random phase approximation including self and exchange contribution to compute the ground state properties at high density $r_s$. Our results demonstrate that the confinement geometry significantly modifies effective electron interactions in one-dimensional (1D) systems. The static structure factor and pair correlation function reveal enhanced density correlations and spatial ordering, particularly signified by a pronounced $2k_F$ peak in the static structure factor and oscillatory behavior of period $2r_s$ in the pair correlation function. As $b \to 0$, the system approaches the idealized 1D system, where interactions dominate resulting in the most negative energies which reflects the stronger correlation effects.

**k0009**

**Systematic Growth of Layered Metallic 1T−$VS_2$ using Chemical Vapor Deposition**

Dipankar Pokhrel[1], Avijit Mahapatra[1], Jaharlal Pati[2], Pamu Dobbidi[1], Malleswararao Tangi[1, a)]
[1]*Department of Physics, Indian Institute of Technology, Guwahati, Assam-781039, India*
[2]*Centre for Nanotechnology, Indian Institute of Technology Guwahati, Guwahati, Assam 781039, India*
[a)]*Email: malli@iitg.ac.in*

Among two-dimensional (2D) layered materials, metallic transition metal dichalcogenides (MTMDCs) have attracted significant interest due to their exceptional electrical conductivity and the recent discovery of room-temperature ferromagnetism, making them promising for applications in electronics, spintronics, and energy-related technologies. In this work, the systematic growth of large-area 1T-$VS_2$ flakes via atmospheric pressure chemical vapor deposition (APCVD) is achieved, with lateral sizes in the range of $15 - 30\ \mu m$. The formation of the predominant 1T-phase is evident with the strong amorphous background, along with the presence of minor $V_5S_8$ as a secondary phase. Electrical characterization reveals linear I–V behavior, validating the metallic nature of the material, with a measured sheet resistance $\sim 20\ k\Omega$. The resistivity, independently evaluated using both geometrical and analytical models, was consistently found in the range of $20 - 40\ \mu\Omega m$. These results demonstrate the growth of crystalline 1T-$VS_2$, with robust metallic electrical performance.

**k0010**

**Graphene-Silver Nanowire-Diamond Substrate for Tunable and Stable Surface Enhanced Raman Spectroscopy Application**

Shweta S. Deshmukh [1, a)] Lekshmi J [1, b)] and Padmnabh Rai[1, c)]
[1]*School of Physical Sciences, UM-DAE Centre for Excellence in Basic Sciences, University of Mumbai, Kalina campus, Santacruz (E), Mumbai 400098, INDIA*
[a)]*Email: shweta.deshmukh@cbs.ac.in*

Diamond, with its exceptional chemical stability and wide bandgap, presents a promising platform for developing robust substrate for Raman signal enhancement. However, in its pristine form, diamond lacks the necessary electromagnetic and chemical activity to support efficient SERS enhancement. In this study, we investigate the impact of graphene layer on SERS performance of silver nanowires (AgNWs) coated diamond substrate. The Raman response of the substrate was evaluated using Rhodamine 6G (R6G) as a probe molecule. The graphene layer over AgNW coated diamond enhances the SERS activity, with an enhancement factor (EF) of $4.4 \times 10^5$. This enhancement arises from the combined effect of electromagnetic enhancement from AgNW and chemical

enhancement provided by graphene on the diamond substrate. Our findings suggest that the combination of graphene with AgNWs on diamond can yield stable and reliable platform for molecular sensing with potential for future gate-tunablility.

**k0012**

**Fe Impurity-Driven Magnetism in 2D-1T'-$MoX_2$ Monolayers: A First-Principles Study**

Dolan Acharya, and J. Karthikeyan
*Department of Physics, National Institute of Technology, Durgapur, West Bengal, 713209, India.*
**Email: da.23ph1104@phd.nitdgp.ac.in*

Since the groundbreaking isolation of single-layer graphene, two-dimensional (2D) van der Waals (vdW) materials have garnered intense research interest due to their exceptional physical properties and potential for next-generation electronic, optoelectronic, and quantum devices. Among these, transition metal dichalcogenides (TMDs)[5] stand out for their polymorphic crystal structures, rich electronic phase space, and the ability to exhibit exotic quantum states not observed in their bulk counterparts. Particularly, unconventional structural phases of TMDs offer expanded tunability in electronic properties, making phase engineering a critical strategy in designing functional devices. In this study, we employ first-principles calculations to investigate Iron (Fe) doping in Molybdenum dichalcogenide $MoX_2$ (X = S, Se, and Te) monolayers,[4] focusing on various defect configurations structural defects isomers such as Interstitial (Int), Substitutional (Sub) and adatom configurations for post growth Fe atom deposition in the 1T′ phases of monolayer (1L-$MoX_2$). Our results indicate that Fe atoms energetically prefer Int-site in the 1T′ phase under X-poor conditions only in ditellurides, inducing strong magnetic moments of 2μB.[1] These findings underscore the potential of atomic-scale impurity engineering to modulate magnetic behavior in 1L-$MoTe_2$, paving the way for tailored functionalities in spintronics, quantum technologies, and energy storage applications.

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**k0013**

**Layer-Dependent Raman Spectroscopy in Graphene**

Memansa Thapa[1]and Ajay Soni[1]*
[1]School of Physical Sciences, Indian Institute of Technology Mandi, Mandi 175005, Himachal Pradesh, India
[*]*Email: ajay@iitmandi.ac.in*

Graphene's physical properties, such as its electrical and mechanical behavior, highly depend on the number of layers. Understanding and accurately determining these layers is therefore crucial for developing next-generation quantum devices. In this study, we have used the non-invasive Raman spectroscopy technique at room temperature to systematically analyze graphene flakes of varying thickness, prepared via mechanical exfoliation of bulk highly oriented pyrolytic graphite (HOPG) onto a $SiO_2$ substrate. The Raman spectra reveal a clear distinction in the G and 2D bands and provide a direct method to accurately identify monolayer, bilayer, trilayer, and multilayer graphene flakes.

**k0014**

**Growth, characterization and x-ray photoemission spectroscopy study of a correlated material, $SmAgSb_2$**

Saswata Halder[1], A. Thamizhavel[1], and Kalobaran Maiti[1,2,*]
*[1]Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai - 400005, INDIA.*
*[2]School of Physical Sciences and School of Materials Sciences, Indian Association for the Cultivation of Science, 2A & 2B Raja S. C. Mullick Road, Jadavpur, Kolkata 700032, INDIA*
**Email: kbmaiti@gmail.com*

We report the growth and characterization of high-quality single crystals of $SmAgSb_2$ using the flux method. $SmAgSb_2$ crystallizes in the layered tetragonal structure *P4/nmm*, which was confirmed using Laue diffraction. It consists of a quasi-two-dimensional structure of Sb atoms which hosts topologically non-trivial fermions. The magnetic susceptibility measurements show high anisotropy with an antiferromagnetic transition temperature $T_N = 9.2$ K. Temperature dependent electrical resistivity measurements at different applied magnetic fields show interesting signature of field induced magnetic structure reorientation /superzone formation. A residual resistivity ratio (RRR) ~ 355 shows the high purity of the grown single crystals. The core-level photoemission spectra of Sm 3*d*, measured using synchrotron radiation, show multiple features resulting from final state effects – a signature of hybridization between Sm 4*f* - Sb 5*p* states. Signatures of surface-bulk difference is observed in the Sb 4*d* core level spectra for different photon energies. These results highlight the significance of depth resolved photoelectron spectroscopy in investigating the surface sensitive electronic structure and complex hybridization physics in correlated materials.

**k0016**

**First-Principles Insights into $ZnO_2$ and $CdO_2$ Monolayers for Thermoelectric and Optoelectronic Applications**

Sajan Yadav[1], Urjitsinh Rathod[2], Sumana Hajra[2], Savan Katba[3], Dheeraj K. Singh[4], Ashish Ravalia[2,a)]

*1. Department of Physics, Saurashtra University, Rajkot 360005, India*
*2. Department of Nanoscience and Advanced Materials, Saurashtra University, Rajkot 360005, India*
*3. Department of Physics, School of Science, RK University, Rajkot-360020, India*
*4. Department of Physics & Astrophysics, Univesity of Delhi, Delhi 110007, India*
*a)Email:* ashishravalia@gmail.com
We present a first-principles study on the thermoelectric and optical properties of two-dimensional (2D) $ZnO_2$ and $CdO_2$ with $MoS_2$-type hexagonal structures. Both materials are indirect semiconductors, exhibiting band gaps of 1.80 eV ($ZnO_2$) and 0.82 eV ($CdO_2$), indicating suitability for photocatalytic and photovoltaic applications. Employing Boltzmann transport theory within the BoltzTrap framework, we assess key thermoelectric parameters, including the Seebeck coefficient, electrical conductivity, and power factor. $ZnO_2$ exhibits superior thermoelectric performance compared to $CdO_2$, underscoring its potential for thermoelectric applications. Optical analyses reveal strong visible-range absorption and partial transparency, indicating potential applicability in optoelectronic devices. These insights contribute to the foundational understanding of $ZnO_2$ and $CdO_2$ and pave the way for their future experimental exploration.

**k0018**

**High Pressure Structural and Resistance Studies on Type-II Dirac Semimetal $Ir_2In_8Se$**

Manisha Yadav[1,2,a)] , Pallavi Malavi[1] and S. Karmakar[1,2]
[1]*High Pressure & Synchrotron Radiation Physics Division, BARC, Mumbai 400085, India*[2]*Department of Physical Science, Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*
**Email: manishay@barc.gov.in*
We present high pressure studies of the structural and electrical properties of type-II Dirac Semimetal candidate $Ir_2In_8Se$ using synchrotron-based x-ray diffraction up to ~20GPa and magneto-transport measurements up to ~12 GPa. The ambient tetragonal structure (SG: *$P4_2/mnm$, $z=4$*) remains stable up to ~5GPa above which the system undergoes reversible structural transition with a lower symmetry orthorhombic structure (SG: *Pnnm, $z=4$*). Our resistance measurements with pressure show that the system remains overall metallic at least up to 11.2GPa, without showing any signature of superconductivity. At ~6GPa an anomalous behavior observed in residual resistivity and RRR along with carrier density and mobility, indicating a possible electronic structural transition associated with structural transition. The polyhedral disorder of $IrIn_8$ in the tetragonal structure occurs at ~183K which is decreases with increasing pressure up to 6 GPa, indicating enhanced intrinsic disorder followed by an anomalous upturn above 6GPa.

**k0021**

**Temperature-dependent Bandgap and Exciton-phonon Coupling in $TlGaS_2$ Single Crystal**

Soumik Bhattacharya, and Durga Basak*
*School of physical sciences, Indian Association for the Cultivation of Science, 2A & B Raja S.C. Mullick Road, Jadavpur, Kolkata 700032, India*
**Email: sspdb@iacs.res.in*
The optical bandgap of quasi-2D $TlGaS_2$ single crystal has been found to be 2.42 (direct) and 2.32 eV (indirect) from the transmission spectra. A detailed investigation on the temperature-dependent optical bandgap and exciton-phonon coupling for $TlGaS_2$ leads to an average phonon energy and the electron-phonon coupling constant values using the O'Donnell and Chen model as $< E_{Ph} > = 33$ meV and S = 4.42 respectively, being reported here unprecedentedly. Further, the coupling strength for both the LO and acoustic phonons are calculated from the temperature-dependent linewidth broadening of the narrow exitonic peak observed in the photocurrent spectra and presented as $\gamma_{LO}$ = 231 meV and $\gamma_{ac}$ = 50 μeV/K respectively. Linearly temperature-dependent acoustic phonons play a crucial role in exitonic transport at low temperature wherein strong LO phonons defining the optical and transport properties of the material at higher temperature.

**k0022**

**Role of Disorder and Spin-orbit Coupling in Tunning the Bulk Type-II Dirac Node in 1T-RhSeTe**

Neeraj Bhatt, Soumyajit Sur, Chandan Patra, Ravi Prakash Singh and Ravi Shankar Singh *)
*Department of Physics, Indian Institute of Science Education and Research Bhopal, Bhopal Bypass Road, Bhauri, Bhopal – 462066, M. P., India*
**Email: rssingh@iiserb.ac.in*
We investigate the effect of disorder at chalcogen site on the electronic structure of 1T-RhSeTe using density functional theory. $RhTe_2$ exhibits bulk type-II Dirac node at about 320 meV above the Fermi level whose energy position can be tuned by substitution of Te with Se modifying the effective spin orbit coupling strength. Our results reveal that the Dirac node in case of RhSeTe appears in the close vicinity of Fermi level. Further phonon band structure reveals signatures of the charge density wave ordering in RhSeTe indicating dimerization similar to other 1T-type transition metal dichalcogenides. Our findings demonstrate that chalcogen site substitution can be an effective strategy to tune both electronic band topology and lattice instabilities in layered transition metal dichalcogenides.

**k0023**

**Role of Electron Correlation in the Surface Electronic Structure of type-II Dirac Semimetal $NiTe_2$**

Neeraj Bhatt, Asif Ali, Deepali Sharma, Sakshi Bansal, Mansi Mandal, Ravi Prakash Singh and Ravi Shankar Singh*
*Department of Physics, Indian Institute of Science Education and Research Bhopal, Bhopal Bypass Road, Bhauri, Bhopal–462066, M. P., India*
**Email: rssingh@iiserb.ac.in*

We investigate the electronic structure of $NiTe_2$ using angle-resolved photoemission spectroscopy and theoretical approaches. While the bulk as well as surface Fermi surface is well described within mean-field approaches, an accurate description of the topological surface state appearing much below the Fermi level necessitates the consideration of strong surface electronic correlation effects. Our study highlights the critical role of many-body interactions in determining the topological surface states in $NiTe_2$, advancing the understanding of electron correlation effects in topological quantum materials.

**k0024**

**An *ab initio* Study of Phosphorene Like Group IV-VI 2D XS (X = C, Si, Ge) Compounds**

Laltha Kimi[1,2,b)] and Lalhriat Zuala[2,a)]
[1] *Department of Physics, School of Physical Science, Mizoram University, Aizawl-796004, Mizoram*
[2] *Physical Sciences Research Center (PSRC), Department of Physics, Pachhunga University College, Mizoram University, Aizawl-796001, Mizoram, India*
[a)]*Email (Corresponding author): hriata@pucollege.edu.in*
[b)]*Email (Presenting author): lalthakimi@pucollege.edu.in)*

Using Density Functional Theory (DFT) calculation, group IV-VI 2-dimensional XS (X = C, Si, Ge) monolayers having phosphorene like configuration were constructed to investigate their structural, electronic, and optical properties. Optimization of the structure results in the increase in volume with the increase in the size of atoms. The compounds are found to be thermodynamically stable. These monolayers are all semiconductors with the band gaps of 1.21~1.685 eV. The calculated optical properties indicate that all compounds exhibit optical absorption in the visible region with low reflectivity lower than 8%. All results suggest that the investigated compounds are promising candidates for optoelectronic devices.

**k0025**

**Polarized Raman Spectroscopy of Tin dichalcogenides $SnS_{(2-x)}Se_x$**

Rachna Selvamani[1,*], Swayam Kesari [1], Rekha Rao[1, 2,*], and M. P. Deshpande[3]
[1]*Solid-State Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, India*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai-400085, India*
[3]*Department of Physics, Sardar Patel University, Vallabh Vidyanagar, Gujarat 388120, India*
**Email: srachna@barc.gov.in; rekhar@barc.gov.in*

Metal dichalcogenides (MDCs) are interesting due to their unique structural characteristics and promising technological applications. The vibrational investigation of a series of single crystals of tin dichalcogenides $SnS_{(2-x)}Se_x$ (x = 0, 0.5,1.0 and 1.5) using Raman spectroscopy is conducted. The successful identification of the symmetries of all the observed Raman modes is conducted using polar plots observed in the polarized Raman spectroscopy. Three Raman peaks are observed at 307 $cm^{-1}$, 205 $cm^{-1}$, and 190$cm^{-1}$ in mixed system $SnS_{(2-x)}Se_x$ (x= 0.5,1.0 and 1.5). The two modes around 205 $cm^{-1}$ and 307 $cm^{-1}$ are identified to be $A_{1g}$ of $SnSe_2$ and $SnS_2$, respectively and are consistent with previous reports. The other mode ~190 $cm^{-1}$ is not $E_g$ type as previously reported but rather is $A_{1g}$ type and may be associated with sulphur-deficient SnS (π-cubic) phase of $SnS_2$.

**k0026**

**Electronic Structure of $In_2Se_3$: An *ab-initio* Study.**

Mitanshi Gupta, Soumyajit Sur, Saswata Talukdar, Surajit Saha and Ravi Shankar Singh[(a)]
*Department of Physics, Indian Institute of Science Education and Research Bhopal, Bhopal Bypass Road, Bhauri, Bhopal-462066, M.P. India*
**Email: rssingh@iiserb.ac.in*

We investigate the electronic structure and dynamical stability of the crystal structure for various polymorphs of $In_2Se_3$ within the framework of density functional theory. Crystal structure of $In_2Se_3$ consist of quintuple layers (Se-In-Se-In-Se) forming *a-b* plane. These quintuple layers are van der Waals bonded and stacked along *c*-axis. The distortion in the quintuple layers lead to different phases (*a* and *b*), while the stacking order along *c*-axis leads to different symmetry (2H and 3R). The *a*-$In_2Se_3$ (2H and 3R) are found to be semiconducting with structural stability, while both 2H and 3R *b*-$In_2Se_3$ show a narrow gap with dynamically unstable structure. Our results highlight the critical role of both stacking order and intralayer atomic coordination/arrangement in governing the structural stability and electronic structure of $In_2Se_3$.

**k0028**

**Low Temperature Surface Conductivity in $SmB_6$: A Two-fluid Perspective**

Sugata Paul[1], Sayantan Ghosh[1], Tamoghna Chattoraj[1], Ritesh Kumar[1], Zachary Fisk[2], S. S. Banerjee[1,a]
[1]*Indian Institute of Technology Kanpur, Kanpur, Uttar Pradesh 208016, India.*

[2]*Department of Physics and Astronomy, University of California at Irvine, Irvine, CA 92697, USA.*
[a]*Email : satyajit@iitk.ac.in*
Samarium Hexaboride ($SmB_6$), a candidate topological Kondo insulator, exhibits sharp rise in resistivity below 30–50 K due to bulk Kondo gap opening, followed by a resistivity plateau below ~5 K— suggesting surface conduction, though its topological nature remains debated. To probe this low-temperature ($T$) behavior, we employ two-coil mutual inductance measurements and identify three temperature regimes: (i) $T \geq T^*$ (~62 K), (ii) $T_g$ (~23 K) $\leq T < T^*$ and (iii) $T < T_g$. We observe that a 2.2 meV 'in-gap' feature hosting light Dirac-like carriers, coexist with heavy quasiparticles released from a disorder-driven Kondo breakdown on the surface. $I - V$ and specific heat measurements confirm this two-fluid behavior, with a distinct surface Kondo temperature $T_k^S \approx 7$ K. Nyquist analysis revealing a transition from high- $T$ pure capacitive to low- $T$ capacitive–inductive response, strengthens the coexistence of light and heavy carriers contributing to low-$T$ non-trivial surface conduction in $SmB_6$.

**k0030**

**Structural, Magnetic and Magneto-Transport Properties of Single Crystalline $Fe_{3+x}GeTe_2$**

Rosni Roy, Sandip Paul, Gourab Kanti Jana, and Rajib Mondal
*UGC-DAE Consortium for Scientific Research, Kolkata Centre, LB-8, Sector III, Bidhannagar, Kolkata 700 106, India*
**Email: rosniroy455@gmail.com*
A comprehensive study including structural, magnetic, magnetocaloric and magnetotransport behavior of van der Waals bonded single crystalline $Fe_{3+x}GeTe_2$ has been carried out. $Fe_3GeTe_2$ crystallizes in hexagonal crystal structure with space group $P6_3/mmc$ (No. 194). The material undergoes a paramagnetic to ferromagnetic phase transition around ~237 K ($T_C$). This work observes a significant conventional magnetocaloric effect with isothermal entropy change -3.2 J/kg-K for 100 kOe magnetic field change. Temperature ($T$)- dependent in-plane resistivity shows metallic behavior present in this material. Electrical and magnetotransport measurements reveal a magnon dominated scattering mechanism in $Fe_{3+x}GeTe_2$. The findings demonstrate that, the material $Fe_{3+x}GeTe_2$ holds great promise as a potential candidate for spintronic applications.

**k0031**

**A First-principles Study of 2D MXene-like $SiSnGeN_4$ For Photocatalytic Applications**

*C. B. Subba[1], B. Chettri[1], L. D. Tamang[1], D. P Rai[1,a)], Z. Pachau[1]*
*[1](Department of Physics, Mizoram University, Aizawl-796004, India)*
**Email: dibyaprakashrai@gmail.com*
The rise of 2D materials has transformed nanoscale technologies. Here, first-principles DFT calculations reveal that a novel $SnSiGeN_4$ monolayer features a wide, tunable band gap, strong in-plane vibrational (XX, YY) modes, and pronounced optical anisotropy. The material exhibits strong UV absorption and minimal ZZ response, making it a promising candidate for UV photodetectors, optoelectronics, and visible-light photocatalysis through band gap engineering.

**k0032**

**Topological Nodal-line Phonons in Ternary KCuX (X = Se, Te) Compounds**

Aiswarya T[1, a)] Andrzej Ptok[2, b)] and G. Vaitheeswaran[1, c)]
*[1] School of Physics, University of Hyderabad, Prof. C. R. Rao Road, Gachibowli, Hyderabad-500046, Telangana, India.*
*[2] Institute of Nuclear Physics, Polish Academy of Sciences, ul. W. E. Radzikowskiego 152, 31-342 Kraków, Poland.*
*Email: [b] aptok@mmj.pl [c] vaithee@uohyd.ac.in*
We report a detailed investigation into the topological phonon properties of ternary potassium copper chalcogenides KCuX (X = Se, Te), which crystallize in a non-symmorphic hexagonal P6_3/mmc structure. Ab initio phonon calculations reveal rich symmetry-driven features, including nodal planes at kz = ±π/c, quadratic contact points, and intricate nodal line networks. These topological features are directly linked to underlying space group symmetries. Our surface phonon spectral calculations reveal unconventional drumhead-like surface states located around the K points. The compounds demonstrate promising characteristics for application in phonon-based information processing and thermal management technologies.

**k0033**

**Photoluminescence study of ZnSe Nanoplatelets**

Amruta Lohar,[1] Shivani Vijay Tiwari,[2] Mohammed Abdul Haque,[1] Shrikrishna D. Sartale,[1] Y. D. Kolekar,[1] Shailaja Mahamuni[1,*]
*[1]Department of Physics, Savitribai Phule Pune University, Pune, Maharashtra, India-411 007*
*[2]Defence Institute of Advanced Technology, Pune, Maharashtra, India – 411025*
**Email: shailajamahamuni@yahoo.co.in*
Two dimensional nano systems have characteristic intense and narrow emission with suppressed inhomogeneous broadening. In the present work, ZnSe nanoplatelets (NPLs) which are rather non-toxic compared to cadmium-based systems are investigated. Two different thicknesses were synthesized using hot-injection chemical route method. The ZnSe NPLs show two sharp and narrow absorption peaks at 347, 329 nm (3.57, 3.76 eV) and 294, 282 nm (4.21, 4.39 eV) for rectangular ZnSe (r-ZnSe) and triangular ZnSe (t-ZnSe) NPLs respectively. The absorption features are attributed to heavy hole-electron (hh-e) and light hole - electron (lh-e) transitions. The difference between the hh-e and lh-e transition decreases from 18 nm (0.19 eV) to 12 nm (0.18 eV) for r-ZnSe

and t-ZnSe NPLs as thickness of NPLs decreases. Photoluminescence (PL) of r-ZnSe NPLs is observed at 349 nm (3.55 eV) with narrow fwhm of 7.1 nm (72 meV). PL emission spectra of r-ZnSe NPLs at 80 K display the presence of surface and point defects. Huang-Rays factor (S factor) which indicates the strength of electron-phonon coupling is 4.5. The exciton binding energy is ~32.6 meV. The presence of localized states is evident from the anomalous temperature dependence of PL emission fwhm. These results signify that there is a strong influence of phonons and localized states on the electronic transitions of r-ZnSe NPLs.

**k0034**

**Transforming $NbOCl_2$ To Janus NbOClBr And Unveiling Its Structural, Electronic, And Optical Properties Via Density Functional Theory**

L. D. Tamang[1,2], Shivraj Gurung[2,3], B. Chettri[1], C. B. Subba[1], L. Celestine[2], R. Zosiamliana[2], N. T. Tien[3], D. P. Rai[1,a)*]
[1]Department of Physics, Mizoram University, Aizawl- 796004, India
[2]Physical Sciences Research Center (PSRC), Department of Physics, Pachhunga University College, Aizawl- 796004, India
[3]College of Natural Sciences, Can Tho University, Can Tho City, Vietnam
[a)]*Email: dibyaprakashrai@gmail.com*

Theoretical and experimental studies of numerous Janus monolayers have discovered interesting novel properties. This study investigates the structural, electronic, and optical properties of Janus NbOClBr monolayer formed by substitutional doping of $NbOCl_2$ with Br atoms within the GGA-PBE approximations. The studied system crystallized in a monoclinic crystal with space group P1. Due to a larger radius of Br atoms, the bond length between Nb-halogen increases by 0.1 Å. The formed system $NbOCl_XBr_Y$ exhibits a band gap between (0.6 – 0.7) eV, which can be further corrected using the existing hybrid functionals. The bonds formed within the system were found to be ionic. These materials can be activated under the visible and UV regions of the solar spectrum.

**k0035**

**Electron-Hole Plasma Optical Gain in Metal Halide Perovskites Quantum Dots**

Naresh Aggarwal[1], Dmitry N. Dirin[2], Maksym V. Kovalenko[2,3], K. V. Adarsh[1a)]
*[1]Department of Physics, Indian Institute of Science Education and Research, Bhopal,462066, India*
*[2]Laboratory of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zürich, CH-8093 Zürich, Switzerland*
*[3]Empa - Swiss Federal Laboratories for Materials Science and Technology, CH-8600 Dübendorf, Switzerland*
**Email: adrash@iiserb.ac.in*

Metal halide perovskites (MHP) quantum dots (QDs) are a promising platform for the lasing and optoelectronic applications due to their exceptional properties. Despite various demonstrations of optical gain in MHP QDs, the role of electron-hole plasma (EHP) phase remains largely unexplored. In this study, we revealed the role of EHP phase in ASE in $CsPbBr_3$ QDs by using temperature and fluence dependent photoluminescence and transient absorption measurements. At 5 K, two ASE bands with the threshold fluences of 25 and 100 $\mu J/cm^2$ corresponding to excitonic and EHP phase are demonstrated respectively. The EHP driven ASE produces a broadband optical gain of ~ 150 meV, indication of strong many body interactions. This dual-band behaviour persists for up to 200 K. At room temperature, this EHP induced ASE behaviour vanished due to the substantial contribution of non-radiative recombination, phonon populations and increased the Mott density threshold. This work demonstrates the potential of EHP to be a practical platform for studying macroscopic quantum phenomena and developing optoelectronic devices.

**k0036**

**Effect of Dimension Reduction on superconducting properties of Aluminum: Ab initio investigation**

Neetesh Cheeta[1,2, a)] and Jagannath[1,2]
*[1]Technical Physics Division, Bhabha Atomic Research Center, Mumbai, 400085*
*[2]Homi Bhabha National Institute, Mumbai,400094*
*[a)] Email:* Neetesh Cheeta (neeteshc@barc.gov.in)

Aluminum (Al) is a well-known superconductor with a superconducting transition temperature of 1.2K in its bulk state. It is a workhorse material for fabrication of superconducting Qubits. Many experimental studies show that dimension reduction from 3D to 2D can extremely change the superconducting properties due to inclusion of Quantum effects. For aluminum it is experimentally observed that in the thin film structures the transition temperature and superconducting gap at fermi level have tendency to increase. In this study, by employing the first principal approaches like density functional theory (DFT) and Density functional perturbation theory (DFPT) we have calculated the superconducting properties of Aluminum in its bulk and monolayer state using Quantum ESPRESSO and EPW (Electron- Phonon coupling using Wannier functions) code. We have calculated the electron-phonon coupling constant ($\lambda$), Eliasberg spectral function ($\alpha^2F(\omega)$), superconducting transition temperature (Tc), superconducting gap ($\Delta$). Our calculation showed that bulk state transition temperature ($T_c$) 1.2K is enhanced to around 7.5K in the monolayer state, which is in good agreement with experimental studies.

**k0037**

**Many Body Correlation Effects in The Cylindrical Confinement of Quasi-One-Dimensional Quantum Wire**

Sudesh Kumar[1], Vidit Gangwar[1], Gautam Shah[1] and Vinod Ashokan[1, *]
*[1]Computational Quantum Many-Body Physics Lab, Department of Physics,*

*Dr. B. R. Ambedkar National Institute of Technology, Jalandhar, Punjab - 144008, India*
**Email: ashokanv@nitj.ac.in*
The many body correlation plays a crucial role in determining the physical properties of quantum materials. Their contribution has critical effect on the strength of the electron-electron coupling parameter $r_s$, which is a characteristic property of the emergent quantum materials. In this work, the electrons are confined in quasi-one dimension by the cylindrical potential. We use dynamical first-order random phase approximation which includes self and exchange-energy contributions to calculate the ground-state properties of quasi-one-dimensional ferromagnetic quantum wire at various wire widths $b$ and density parameters $r_s$. We numerically calculated the pair-correlation function, static structure factor, and correlation energy at high-density. The pair-correlation function shows oscillatory behaviour for different $r_s$ with the highest peak at higher value of coupling parameter. The $2k_F$ peak height of the static structure factor grows as $r_s$ increases, indicating increased electron-electron correlation. We have also observed that the correlation energy converges to $-\pi^2/360$ for ultra-thin wire in the high-density regime ($r_s \leq 1$), which is in agreement with the exact high-density theory and quantum monte Carlo simulation.

**k0038**

**Wurtzite LiZnAs as Composite Quantum Compound with Hyperferroelectricity, Rashba Effect and Topological Phases**

Saurav Patel[1, *], Paras Patel[1], Shaohui Qiu[2] and Prafulla K. Jha[1]
[1]*Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, India-390002.*
[2]*Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701, USA.*
**Email: sauravpatel317@gmail.com (Email of corresponding author)*
This work establishes a density functional theory (DFT) based predictive framework for identifying composite quantum compounds (CQCs) that exhibit intertwined hyperferroelectricity (HyFE), multiple topological phases and giant Rashba spin splitting (RSS). We studied the role of spin-orbit coupling and crystalline symmetries in LiGaGe-type LiZnAs polar compound. The phonon dispersion curves and rigorous electric free energy analysis confirm the intrinsic HyFE nature of LiZnAs, exhibiting a giant polarization of 0.28 C/m² under open-circuit boundary conditions (0.75 C/m² under short-circuit conditions) and a deep free energy well of –66 meV which is largest reported to date among intrinsic HyFE materials. A strain-driven topological phase transition (TPT) from a trivial insulator to a Weyl semimetal at critical point and eventually a topological insulator phase (TI) is achieved under moderate biaxial strain of 3.4%. The relativistic band structure along M–Γ–K path reveals significant Rashba coefficient of 5.91 eV Å for Weyl semimetal phase while 2.43 eV Å for TI phase. The Z2 topological invariants and Berry curvature confirm the topological nature. Our findings present a unified framework for designing HyFE Rashba semiconductors with tunable topological functionalities, paving the way for their integration in next-generation spintronic and quantum devices.

**k0039**

**Exploring Spin textures and Modulating Spin-Splitting in Layered Perovskites: A First-Principles Computational Approach**

Shantanu Pathak[1, a)] and Saswata Bhattacharya[1, b)]
[1]*Department of Physics, Indian Institute of Technology Delhi, New Delhi, 110016, India*
*Email:* [a)]shantanu.pathak@physics.iitd.ac.in; [b)] saswata@physics.iitd.ac.in
Noncentrosymmetric materials (lacking inversion symmetry) exhibit electronic energy bands splitting by the Spin-Orbit Coupling (SOC) effect. This effect is responsible for non-trivial spin configurations and emergent quantum mechanical phenomena. Persistent spin texture (PST) refers to the ability of certain materials to uphold a consistent spin configuration across momentum space. This characteristic is anticipated to contribute to significantly prolonged carrier spin lifetimes, holding great potential for spintronics applications. Here, we predict this property in a noncentrosymmetric orthorhombic family of layered organic-inorganic lead halide perovskites. In the material, the PST property is enforced by nonsymmorphic space group symmetry. We study this behavior in $A_2BX_4$ (A = organic ammonium cations, B = Pb, Sn, X = Br, I) perovskites using density functional theory (DFT). We investigate spin-dependent electronic structures and demonstrate the appearance of spin configurations as PST driven by spin-orbit coupling. We observe large spin-splitting at the conduction band minimum around ~3.3 eV·Å and PST around the conduction band minima and valence band maxima in the $k_x$–$k_y$ path for our materials. This spin splitting occurs due to the contributions of Pb-5d and I-5p orbitals in the upper valence band and lower conduction band of the material. The two-band $\boldsymbol{k \cdot p}$ model is used to analyze spin configurations in terms of PST and validate the results obtained using DFT. Further, we study the tuning of spin splitting by applying strain or stress on the materials. Our findings expand the variety of materials that can be employed for spintronics applications.

**k0040**

**Behavior of Interacting Electrons in an AB Ring with Correlated Disorder: A Mean Field Study**

Rahul Samanta[1,a)] and Santanu K. Maiti[1,b)]
*Physics and Applied Mathematics Unit, Indian Statistical Institute,*
*203 Barrackpore Trunk Road Kolkata- 700 108, India*
*Email: rahulsamanta053@gmail.com*[1,a)] *and santanu.maiti@isical.ac.in*[1,b)]
We investigate the role of on-site Hubbard interaction on persistent current in an isolated quantum ring with Aubry-type quasi-periodic disorder in the half-filled band regime, using a Hartree-Fock mean-field approach. We construct the Hamiltonian within a tight-binding framework and numerically investigate the combined effect of correlated disorder and on-site interaction. Our results

reveal that the Hubbard interaction enhances the current when disorder is introduced in the on-site energies while the hopping remains uniform. In contrast, introducing disorder in the hopping suppresses the current with increasing interaction, and this suppression becomes more pronounced at higher disorder strength. When both on-site and hopping disorders are present, the current increases with interaction, with stronger enhancement observed when on-site disorder dominates; the rate of enhancement diminishes as the disorder strengths are comparable.

**k0041**

**Anomalous Circular Currents and Drude Weight in an SSH Ring with Higher-Order Hopping and Disorder**

Sourav Karmakar[1, a)] and Santanu K. Maiti[1, b)]
*Physics and Applied Mathematics Unit, Indian Statistical Institute, 203 Barrackpore Trunk Road, Kolkata-700 108, India.*
*Email: [a)]karmakarsourav2015@gmail.com and [b)]santanu.maiti@isical.ac.in*

The present work investigates flux-driven circular charge current in a Su-Schrieffer-Heeger (SSH) ring in presence of higher order electron hopping within a non-interacting electron picture. Illustrating the system using a tight-binding framework, we compute circular current following the well-known derivative method. In presence of higher order hopping, several anomalous signatures are found that are studied critically. We also inspect the conducting behavior by analyzing Drude weight as a function of disorder.

**k0042**

**Spin-selective Electronic Specific Heat in a Magnetic System**

Sanchita Nandi[1, a)] and Santanu K. Maiti[1, b)]
[1]*Physics and Applied Mathematics Unit, Indian Statistical Institute*,
*203 Barrackpore Trunk Road, Kolkata-700 108, India*
*Email:* [a)]*sanchitanandi208@gmail.com* and [b)] *santanu.maiti@isical.ac.in*

We explore spin-specific electronic specific heat (ESH) in a magnetic chain within a tight-binding framework. A significant enhancement of ESH is observed with increasing the spin-dependent scattering factor. Determining up and down spin ESHs, we also estimate spin polarization (SP), and find a high degree of SP in a wide range of electro-chemical potential. Our analysis provides a new route of estimating thermal response in different magnetic systems.

**k0043**

**Magnetic Property of spin dimer $CrFeTeO_6$**

*Mayuri Kamble [1*], P D Babu[1], and Rimpi Dawar[2]*
[1]*UGC- DAE Consortium for Scientific Research, Mumbai Centre, BARC Campus, Mumbai- 400085, INDIA*
[2]*Bhabha Atomic Research Centre, Chemistry Division, HBNI, Mumbai-400085, INDIA*
**Email: mayucsr@gmail.com*

The polycrystalline $CrFeTeO_6$ is synthesized by solid state method and characterized by x-ray and neutron power diffraction. Rietveld refinement confirms the single phase with space group *P42/mnm,* inverted trirutile type structure with Tetragonal crystal lattice. Magnetization measurements reveal that compound orders antiferromagnetically at 196 K and no anomaly is observed in specific heat around $T_N$ Very small value of 9T magnetic moment even at lowest temperature indicate strong antiferromagnetic coupling $Cr^{+3}$-$Fe^{+3}$ form heteronuclear dimer spins. Results suggest complex magnetic structure.

**k0045**

**Dual-Gate Bias Driven Tuning of Electrical Behaviour of $MoS_2$ FET**

Samiksha[1,*] and Pramod Kumar[1]
[1]*Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India*
**Email: samikshabhatia@iitb.ac.in*

Controlling charge carrier transport in Molybdenum Disulfide ($MoS_2$) field-effect transistors (FETs) is crucial for enabling their integration into next-generation 2D based nanoelectronics devices. Here, we demonstrate effective transport control using a dual-gated FET with sputter deposited $SiO_2$ as top gate dielectric. To evaluate, we first analyse the back-gated performance of FET under various fixed top gate biases ($V_{tg}$). As $V_{tg}$ increases from 0 to 3 V, threshold voltage ($V_{th}$) changes from 19 to 3.6 V and on state current ($I_{on}$) increases from $3.85\times10^{-6}$ to $1.07\times10^{-5}$ A, indicating tuning of $V_{th}$ and enhanced channel conductivity. Conversely, the top-gated performance of FET is analysed under various fixed back gate biases ($V_{bg}$). As $V_{bg}$ increases from 0 to 3 V, $V_{th}$ changes from 2.27 to 1.91 V, $I_{on}$ increases from $1.25\times10^{-6}$ to $2.17\times10^{-6}$ A. These results confirm efficient electrostatic coupling between the top and back gates, offering dynamic control over channel conduction and demonstrates the promise of dual-gated architectures for threshold-voltage tuning and improved electrical performance through higher drive currents.

**k0046**

**Topological Signatures and WAL-WL Transition in Cr-Doped $Bi_2Se_3$ on STO (100)**

Vishal K Maurya[1,*], Sudhanshu Gautam[2], Rahul Kumar[1,3], S.S. Kushvaha[1]
[1]*CSIR-National Physical Laboratory, Dr. K.S. Krishnan Marg, New Delhi 110012, India*
[2]*Institute Instrumentation Center, Indian Institute of Technology Roorkee, Roorkee Uttarkahand, 247667 India*
[3]*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad 201002, India*
**Email: mauryavishal1@gmail.com*

We have deposited thin films of $Bi_2Se_3$ and Cr (18%) doped $Bi_2Se_3$ on $SrTiO_3$ (STO) (100) substrate using RF and DC magnetron sputtering technique. The XRD reveals prominent peaks are aligned in the (0003*l*) direction, which indicates the growth is highly oriented towards the crystal c-axis. Raman spectroscopy has confirmed that both the pure and Cr-doped $Bi_2Se_3$ thin films on STO (100). The broadening of the peaks in the Cr-doped sample suggests that the introduction of dopants has caused some distortion in the lattice. We investigated magneto-transport properties down to 2 K under perpendicular magnetic fields ranging from –14 to +14 T. The weak anti-localization (WAL) effect and its crossover to weak localization (WL) were analyzed in both pristine and Cr-doped $Bi_2Se_3$ films. Dephasing length ($L_\Phi$) and the number of independent transport channels ($\alpha$) were extracted using the modified Hikami–Larkin–Nagaoka (HLN) model at 2, 5, 10, 20, 50, and 100 K temperatures. The fitting parameters give the highest coherence length $L_\varphi$ value of 206 nm at 5 K in pristine $Bi_2Se_3$ thin films. We have observed $\alpha$ value in the range of -0.6 to -0.8, which suggests a single surface transport channel in thin films.

**k0048**

**Electronic and Optical Properties of 2D Monolayer Superhard Material from First Principles Study**

Gadha R. J and R. D. Eithiraj
Department of Physics, School of Advanced Sciences, Vellore Institute of Technology, Chennai-600 127, Tamil Nadu, India.
*Email: eithiraj.rd@vit.ac.in

In this work, using first principles calculations, the structural, electronic and optical properties of monolayer sodium rhenium nitride ($NaReN_2$) was investigated. The monolayer crystallizes in a trigonal symmetry and possesses metallic behaviour as unveiled by its band structure. In depth analysis of its optical response, comprising of absorption coefficient, reflectivity and refractive index has been performed to highlight its possibility for optoelectronic and photonic applications.

**k0050**

**First-Principles Study of Kagome Metal EuV3Sb4**

D. Gurung[1],R. Tamang[1], D. P. Rai[1, a)]
*1) Department of Physics, Mizoram University, Aizawl-796004, India*
*[a)]Email: dibyaprakashrai@gmail.com*

We present the first density functional theory investigation of the Fmmm Kagome-lattice compound $EuV_3Sb_4$ using FPLO-PBE calculations. The structure consists of Eu zigzag layers interleaved with V-Sb networks, where V atoms form a two dimensional Kagome framework. The scalar relativistic band structure reveals a metallic ground state with flat-band like features and Dirac-like crossings from Kagome derived states. The Spin resolved analysis shows distinct majority and minority channels, while the Fermi surface is seen to host quasi-2D cylindrical sheets around the Γ point and hexagonal like pockets around the boundaries. The strong angular variation of extremal orbits highlights pronounced two dimensionality, establishing $EuV_3Sb_4$ as a promising platform for exploring magnetically driven topological phases.

**k0051**

**Superhydrophobic Nickel-Graphene Hybrid Coating: A Scalable Approach For Long-Term Corrosion Protection Of Copper**

Pushp Raj Harsh[1(a)], Ujjwal Prasad[1], S. R. Kumar[2], N. B. Chaure[3] and K. Prasad[1]
*[1]University Department of Physics, T. M. Bhagalpur University, Bhagalpur, 812007, India*
*[2]Department of Applied Science and Humanities, NIAMT, Hatia, Ranchi, 834003, India*
*[3]Department of Physics, Savitribai Phule Pune University, Pune, 411007, India*
**Email: pushprajharsh@gmail.com*

The present work focuses on the environmentally friendly fabrication of Ni–graphene (Ni–G) coatings on copper substrates via the electrodeposition method. Surface morphology, examined through SEM, revealed a coarser texture associated with the incorporation of graphene. Potentiodynamic polarization studies were conducted to evaluate corrosion current density and corrosion resistance. The results demonstrate that the Ni–G coatings exhibit enhanced microhardness and superior corrosion resistance compared to bare copper. This improvement is attributed to the high specific surface area of graphene, the presence of electrochemically generated few-layer graphene with high electrical conductivity, its excellent barrier properties that limit water uptake and ion permeation, and the uniform dispersion of Ni–G throughout the coating matrix**.**

**k0052**

**Structural and Electronic Properties of Gold: An Ab-initio study of Bulk, 2D and 1D Phases.**

Poonam Bharti[1,a)], Amandeep Kaur[1], Sheetal[1], Sheetal Dhiman[1], Monika Chandel[1], Surjeet Chandel[1], Anjna Devi[2], Arun Kumar[1]
*[1]Govt. College Bilaspur, Himachal Pradesh, India, 174001*
*[2]Government degree college Baroh, Kangra HP, India, 176054*
**Email: poonambhartisurya@gmail.com*

Gold behaves quite differently at the Nano-scale than its bulk form. While bulk gold is chemically inert, its low-dimensional forms can show high reactivity, even can act as catalysts. We have explored the structural and electronic properties of gold in 3D (bulk), 2D (Goldene and hexagonal-2D monolayer) and 1D (Nano-ribbon) forms. The 1D gold Nano-ribbons demonstrated lower binding energies compared to their bulk and 2D counterparts, indicating higher chemical reactivity and potential for functionalization. Phonon dispersion analysis revealed the absence of imaginary frequencies in all forms indicating the thermally stability of the

studied systems. Additionally, the electronic band structures showed no bandgap, which means they exhibit metallic behaviour. Among the 1D nanoribbons, the 8-AuEneNR$_y$ structure exhibited a magnetic moment of around 0.38μB due to spin splitting and edge effects and can be used in spintronic applications. Overall, our findings show that low-dimensional gold structures hold promise for future Nano-electronic and magnetic devices.

**k0053**

**Field Induced Behavior of the Spin-1 Corrugated Skew-Chain Antiferromagnet: $Ni_2V_2O_7$**

Koushik Chakraborty,[1a] Hemant Singh Kunwar[1], Aditi Agrawal,[1] Isha,[1] Suman Karmakar[1] and Arvind Kumar Yogi[1]
[1]*UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, India*
**Email: koushik7455@gmail.com*

We report the detailed structural, magnetic properties of $Ni^{2+}$ spin-1 corrugated skew-chain $Ni_2V_2O_7$ compound by using of x-ray diffraction, *dc*-susceptibility, magnetization and heat-capacity. The bulk measurements suggest a long-range (LRO) antiferromagnetic ordering at $T_{N1}$ = 6.7 K and $T_{N2}$ = 5.8 K. However, a broad peak centered at around $T_{max}$ ~ 100 K in the $C_P/T$ data along with the divergence of the susceptibility from Curie-Weiss behavior indicates the formation of short-range magnetic correlations ~100 K, which is well above $T_{N1}$. The temperature-dependent x-ray diffraction analysis suggests Ni-Ni bond shortening and $NiO_6$ octahedral distortion significantly below ~100 K. Moreover, the extracted effective moment from our inverse susceptibility Curie–Weiss fit reveals a nearly divalent $Ni^{2+}$ ion moment as ~3.25(3) $\mu_B$, and a Curie-Weiss temperature was found to be $\theta_{CW}$ = -26.4 K, confirming dominant interactions are in antiferromagnetic nature. Interestingly, the system shows field-induced LRO suppression and magnetic ordering has been fully suppressed by the application of a magnetic field at or above 5 Tesla as confirmed by the field-dependent heat capacity.

**k0054**

**Lattice-Electronic Locking and Disorder-Driven Mott Gap Variations in 1T-$TaS_2$**

Soumen Giri[1], Mrinal Manna[1], Pramod Bhakuni[1], Sajal Barman[1], Koushik Chakraborty[1], Aditi Agrawal[1], Arvind Yogi[1], Rajamani Raghunathan[1], Sudipta Roy Barman[1], Rajib Batabyal[1, a)]
[1]*UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore 452001, India*
[a)]*Email:* rajibbata@csr.res.in

We use low-temperature scanning tunneling microscopy/spectroscopy (STM/S) to investigate the interplay between lattice order, electronic correlations, and disorder in the commensurate charge density wave (CCDW) phase of 1T-$TaS_2$. Atomically resolved imaging confirms the ($\sqrt{13}\times\sqrt{13}$)R13.9° "Star of David" (SOD) superstructure and a Mott gap of ~0.38 eV. Structural imperfections induce nanoscale variations in the Hubbard peak positions and, in extreme cases, a collapse of the Mott gap, indicating local breakdown of CCDW coherence. Within the Mott gap, 2D LDOS mapping reveals periodic modulations commensurate with the SOD periodicity, providing direct evidence of Bloch states inside the gap and further demonstrating that surface imperfections can suppress or even eliminate the gap.

**k0055**

**Thermoelectric coefficient in Graphene and Non-relativistic Systems**

Subhalaxmi Nayak, Sabyasachi Ghosh, and Sesha Vempati
*Indian Institute of Technology Bhilai, Bhilai, Chhattisgarh-491002, India.*
**Email: subhalaxmin@iitbhilai.ac.in.*

The present investigation provides a comprehensive analysis of the thermoelectric coefficients, such as Peltier and Thomson effects, within the context of the hydrodynamic behavior of charge carriers in the graphene system. Using kinetic theory formalism with the Boltzmann transport equation under relaxation time approximation, we observe distinct thermoelectric coefficients in the graphene system at room temperature, as compared to the non-relativistic metallic system. Under hydrodynamic conditions near the charge neutrality point, deviations arise in the fluid-based expression for the Peltier and Thomson effects in graphene, distinguishing them from the non-relativistic counterparts.

**k0056**

**Borophene Quantum Dots as Fluorescent Nanosensors for Toxic $Hg^{2+}$ Metal Ion Detection**

H.J. Yashwanth[1*], M. Madhukar Naik[2], H B Shivaprasadh[1], K N Narasimha Murthy[3] Kavyashree D[4]
[1]*Nitte Meenakshi Institute of Technology, Nitte(Deemed to be university) Bengaluru 560107, India*
[2]*Department of Chemistry, BMS Institute of Technology & management, Bengaluru 560107, India*
[3]*Department of Physics, Government First grade college, Bangalore, 560064, India*
[4]*Department of Physics, Acharya Institute of Technology, Bengaluru 560107, India*
**Email*: yashwanthhj95534@gmail.com

Borophene quantum dots (BQDs) were synthesized using a facile liquid-phase exfoliation method and characterized for their structural and sensing properties. X-ray diffraction (XRD) analysis confirmed the nanoscale crystalline features of the BQDs with broad peaks indicating their quantum-confined nature. Fourier-transform infrared (FTIR) spectroscopy revealed the presence of hydroxyl and boron–oxygen functional groups, facilitating water dispersibility and interaction with metal ions. The BQDs exhibited strong blue fluorescence, which was selectively quenched in the presence of toxic $Hg^{2+}$ ions. A pronounced decrease in fluorescence intensity with increasing $Hg^{2+}$ concentration was observed, enabling quantitative detection. The developed BQD-based fluorescent

sensor demonstrated high selectivity and a low detection limit for $Hg^{2+}$, highlighting its potential for environmental monitoring of mercury contamination.

**k0057**

**Effect Of Cuts Introduced In Cellulose Paper, On The Performance Of Graphene/cellulose Paper Pressure Sensors**

Prasad T. Waman[1,2], Devi Prasd Dash[3], Rekha Rao[2,4] and N. Padma[1,2,a)]
[1]*Technical Physics Division, Bhabha Atomic Research Centre, Mumbai, 400085*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai, 400094*
[3]*Veer Surendra Sai University of Technology, Burla, Sambalpur, 768018, Odisha*
[4]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai, 400085*
**Email: padman@barc.gov.in*

Performance of piezoresistive pressure sensors, fabricated by sandwiching graphene nanoplatelets (GNP) coated cellulose papers between two copper plates, was studied. Certain number of cuts (2 and 5) were introduced in cellulose papers before coating with GNP and the performance of pressure sensors using such cut cellulose papers were compared with that of uncut cellulose papers. Pressure sensors using uncut and 2 cuts cellulose papers showed nearly linear increase in response for applied pressure of around 1-10 kPa, with increase in sensitivity (0.55 $kPa^{-1}$) for latter than for former (0.38 $kPa^{-1}$). The sensors with GNP coated 5 cut cellulose papers showed non-linear response, offering higher sensitivity of about 0.65 $kPa^{-1}$ upto 4 kPa and reducing to 0.26 $kPa^{-1}$ beyond this pressure. The increase in sensitivity for pressure sensors with cut cellulose papers than for uncut paper is attributed to the possible deformation in the paper introduced due to cuts in the same, as well as due to improved conducting path through GNP coating at the edges of the cuts. GNP coated 2 cut cellulose paper sensors also showed excellent cyclic stability (~85 % retention) at 10 kPa over 250 cycles and a fast response and recovery time of 80 ms and 60 ms, respectively.

**k0058**

**Enhanced Photodetection Properties of Fe-doped $SnSe_2$ Single Crystal**

*Aarti Lakhara[1], P. A. Bhobe[1]*
*Department of Physics, Indian Institute of Technology Indore, Simrol, Indore 453 552, India)*
**Email: pbhobe@iiti.ac.in (Email of corresponding author)*

We present here a study of photoconductivity properties of $SnSe_2$ and Fe-doped $SnSe_2$ single crystals prepared by chemical vapor transport method. Raman spectroscopy measurement reveals pure phase and effective incorporation of Fe into $SnSe_2$ lattice. The I-V curve measurement of each composition reveals a decrease in resistance consistent with decrease in band gap with Fe-doping. Photo responsivity and external quantum efficiency are found to increase with increasing Fe-concentration, hinting an excellent photodetection application.

**k0059**

**Trimer based hexagonal perovskites: a promising route to quantum spin liquid**

Abhisek Bandyopadhyay[1,2,*], S. Lee[3], D. T. Adroja[1,4], G. B. G. Stenning[1], A. Berlie[1], M. R. Lees[5], and Kwang-Yong Choi[6]
[1]*ISIS Neutron and Muon Source, STFC, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, United Kingdom,*
[2]*Department of Physics, Ramashray Baleshwar College (A Constituent Unit of L. N. Mithila University, Darbhanga), Samastipur, Bihar 848114, India,*
[3]*Center for Artificial Low Dimensional Electronic Systems, Institute for Basic Science, Pohang 37673, Republic of Korea,*
[4]*Highly Correlated Matter Research Group, Physics Department, University of Johannesburg, Auckland Park 2006, South Africa,*
[5]*Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom,*
[6]*Department of Physics, Sungkyunkwan University, Suwon 16419, Republic of Korea*
[*]*Email: abhisek.ban2011@gmail.com*

Frustrated magnets offer a plethora of exotic magnetic ground states, including quantum spin liquids (QSLs), in which enhanced quantum fluctuations prevent a long-range magnetic ordering of the strongly correlated spins down to lowest temperature. Here we have investigated the trimer based mixed valence hexagonal rhodate $Ba_4NbRh_3O_{12}$ using a combination of dc and ac magnetization, electrical resistivity, specific heat, and muon spin rotation/relaxation (μSR) measurements. Despite the substantial antiferromagnetic exchange interactions, as evident from the Weiss temperature ($\theta_W \sim -35$ to $-45$ K), among the Rh-local moments, neither long-range magnetic ordering nor spin freezing is observed down to at least 50 mK, in ac-susceptibility, specific heat, and zero-field μSR measurements (down to 0.26 K). We ascribe the absence of any magnetic transition to enhanced quantum fluctuations as a result of geometrical frustration arising out of the edge-sharing equilateral Rh-triangular network in the structure. Our longitudinal-field μSR results evidence persistent spin fluctuations down to 0.26 K, thus stabilizing a dynamic QSL ground state in Ba4NbRh3O12. Furthermore, the magnetic specific heat data at low-*T* reveal a significant *T*-linear contribution plus a quadratic *T* dependence, which may indicate the gapless Dirac QSL phenomenology of the spinon excitations with a linear dispersion. [1]

References:

[1] A. Bandyopadhyay et al Physical Review B **109**, 184403 (2024) DOI:10.1103/PhysRevB.109.184403

# t) THESIS PAPERS

**t0002**

**Nonlinear Optical Phenomena and Room-Temperature Carrier Dynamics in Nanoscale Materials: Insights and Applications**

Ankit Sharma[1 a)], K. V. Adarsh[1]
[1]*Department of Physics, Indian Institute of Science Education and Research, Bhopal, 462066 India.*
[a)]*Email: ankits19@iiserb.ac.in*

The intricate interplay between nonlinear optical phenomena and ultrafast carrier dynamics stands at the forefront of contemporary research, driven by their transformative potential to shape next-generation optoelectronic technologies. This study highlights the urgent need for materials platforms that can exhibit strong light-matter interactions under ambient conditions. Through detailed optical investigations of advanced material systems, including spinel transition metal oxides, transition metal diselenides, and lead halide perovskites, we elucidate key physical mechanisms that govern nonlinear absorption, refractive index modulation, and coherent emission dynamics. Utilizing techniques such as Z-scan, transient absorption spectroscopy, and time-resolved photoluminescence, we demonstrate the broad applicability of our findings across diverse nanoscale platforms. Our results lay the foundation for novel strategies in the design and control of functional optoelectronic devices that operate at room temperature.

**t0003**

**Emergent Phases, Unconventional Magnetotransport and Magnetic Anisotropy in a Quasi-2D Ferromagnet $Fe_4GeTe_2$**

Riju Pal[1, 2, 3], Buddhadeb Pal[1], Joyal J. Abraham[2, 3], Suchanda Mondal[4], Rajesh O. Sharma[5], Tanmoy Das[5], Bernd Büchner[2, 3], Vladislav Kataev[2, 3], Prabhat Mandal[1], Alexey Alfonsov[2, 3] and Atindra Nath Pal[1]
[1]*Department of Condensed Matter and Materials Physics, S. N. Bose National Centre for Basic Sciences, Block JD, Sector III, Salt Lake, Kolkata, 700106, India.*
[2]*Leibniz Institute for Solid State and Materials Research, Helmholtzstr. 20, D-01069 Dresden, Germany.*
[3]*Institute for Solid State and Materials Physics, TU Dresden, D-01062 Dresden, Germany.*
[4]*Saha Institute of Nuclear Physics, HBNI, 1/AF Bidhannagar, Calcutta 700064, India.*
[5]*Department of Physics, Indian Institute of Science, Bengaluru 560012, India.*
*Email: rijupal07@gmail.com*

Nontrivial spin textures driven by strong exchange interaction, magneto-crystalline anisotropy and electron correlations in low-dimensional magnetic materials often led to unusual electronic transitions. Through a combination of transport experiments and first-principle calculations, we unveil new electronic phases in quasi-2D ferromagnet $Fe_4GeTe_2$ (F4GT) with $T_C \sim 270$ K and spin reorientation ($T_{SR} \sim 120$ K) with the change of magnetic easy axis. Two electronic transitions are identified. The first transition near $T_{SR}$ exhibits a sharp resistivity drop, sign change in the ordinary Hall coefficient ($R_0$), maximum negative magnetoresistance (MR) and anomalous Hall conductivity. Another unusual electronic transition, is observed near $\sim 40$ - 50 K ($T_Q$) featuring positive MR, $T^2$-resistivity, and another $R_0$ sign change. Electron spin resonance (ESR) spectroscopy provides quantitative insights into the non-trivial temperature evolution of the magnetic anisotropy (MA) in F4GT, dominated by demagnetization effect at high temperatures and progressively increased by intrinsic MA below $T_{shape} \approx 150$ K. Below $T_Q$, the intrinsic MA becomes more complex. The consistent signatures in transport and ESR in F4GT confirm an inherent coupling between magnetic and electronic degrees of freedom, emphasizing its relevance for spintronic applications.

**t0004**

**Microscopic Diffusion Mechanism in Lipid Membranes**

Jyoti Gupta[1,2, a)]
[1]*Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai, 400085*
[2]*Homi Bhabha National Institute, Mumbai, 400094*
[a)]*Corresponding author: guptajyoti3024@gmail.com*

Lipid membranes serve as model systems, where lipid diffusion influence signaling, trafficking, and drug delivery. This thesis provides the understating of dynamics of various lipid systems across different membrane phases, including negatively charged (bacterial-like) and zwitterionic (mammalian-like) membranes. Furthermore, it also explores the dynamics of positively charged membranes used in gene therapy, providing insights to improve drug delivery. Neutron scattering techniques is used to study lipid membrane dynamics and their modulation by antimicrobials like ionic liquids (ILs). Additionally, we explored how ILs modulate the dynamics of drug carriers. Our findings reveal that charged lipids exhibit anomalous phase behavior. ILs were found to enhance lipid mobility, modulate drug carriers, and disrupt bacterial membranes by forming nanodomains. Overall, this thesis enhances our understanding of membrane dynamics and antimicrobial interactions, with implications for biology and drug delivery.

**t0005**

**Investigating the intricate magnetism and magnetoelectric coupling induced adiabatic temperature changes in $Fe_2(MoO_4)_3$ and magnetocaloric-ferroelectric behavior in $Tb_2(MoO_4)_3$ compounds**

Athira P[1]
[1] *Department of Physics, NIT Andhra Pradesh, Tadepalligudem, 534101, India*
**Email: athirapganesh@gmail.com*

This study explores the structural, magnetic, and multiferroic properties of rare-earth (RE = Gd, Tb) and transition metal (TM = Fe) based molybdates with the formula $(RE/TM)_2(MoO_4)_3$. $Fe_2(MoO_4)_3$, synthesized via the solid-state method, exhibits a

monoclinic structure ($P2_1/a$) and L-type ferrimagnetic behavior. Magnetic studies revealed a metamagnetic transition ($H_{C2}$) beyond the known multiferroic boundary ($H_{C1}$) and re-entrant spin-glass behavior below $T_{N1}$. Magnetocaloric, electrocaloric, and magnetoelectric-induced multicaloric effects were observed, indicating temperature- and field-dependent cooling—highlighting its potential in low-temperature solid-state refrigeration, tunable near liquid helium temperatures. $Gd_2(MoO_4)_3$ and $Tb_2(MoO_4)_3$ crystallize in orthorhombic β'-phase (*Pba*2) and show promising magnetocaloric performance. $Gd_2(MoO_4)_3$ achieved a high $-\Delta S_m$ of ~31.11 $Jkg^{-1}K^{-1}$ and $\Delta T_{adi}$ of 12.8 K, outperforming $Tb_2(MoO_4)_3$ ($-\Delta S_m$ = 16.78 $Jkg^{-1}K^{-1}$, $\Delta T_{adi}$ = 9.8 K). Both exhibit negligible hysteresis and good field response, making them suitable for cryogenic applications. $Tb_2(MoO_4)_3$ also shows a ferroelectric phase transition at 436 K, supported by dielectric, polarization, and Raman studies, confirming relaxor-like behavior. Its stable dielectric permittivity, low loss, and room-temperature polarization suggest potential in multifunctional applications. Overall, RE molybdates demonstrate strong promise for advanced solid-state refrigeration technologies.

**t0008**

**Spin Pumping With Quantum Materials**

Abhisek Mishra[1] and Subhankar Bedanta[1,2,a)]

*[1]Laboratory for Nanomagnetism and Magnetic Materials, School of Physical Sciences, National Institute of Science Education and Research (NISER), An OCC of Homi Bhabha National Institute (HBNI), Jatni 752050, India.*

*[2]Center for Interdisciplinary Sciences (CIS), National Institute of Science Education and Research (NISER), An OCC of Homi Bhabha National Institute (HBNI), Jatni 752050, India.*

*[a)]Email: sbedanta@niser.ac.in*

Spintronics leverages the spin of electrons to enable faster, energy-efficient, and non-volatile memory technologies. A key challenge is about the efficient generation and detection of pure spin currents. Unlike conventional magnetic memory that requires high magnetic fields, spin-orbit torque magnetic random-access memory uses spin currents, generated via the spin Hall effect in high spin-orbit coupling (SOC) materials, to switch magnetization without external fields. However, reliance on scarce heavy metals like Pt, motivates the search for alternative materials. This thesis explores quantum materials $MoS_2$ (a transition metal dichalcogenide), $Bi_2Se_3$ (a topological insulator), and $RuO_2$ (an altermagnet) for spintronic applications. Using spin pumping, we evaluated their spin transport properties. Large-area $MoS_2$ thin films grown by magnetron sputtering exhibited a spin Hall angle ($\theta_{SHA}$) of 0.02 and a spin diffusion length ($\lambda_{sd}$) of 7.8 nm. Introducing a Cu spacer significantly enhanced the spin Hall angle to 0.30. $MoS_2$ also induced in-plane anisotropy in isotropic CoFeB, likely due to interfacial hybridization. $Bi_2Se_3/Co_2FeAl$ (CFA) heterostructures showed effective spin pumping ($\theta_{SHA}$ = 0.048, λsd = 5.6 nm), with surface-state-induced anisotropy in CFA maximized at 4 nm of $Bi_2Se_3$ thickness. A Cu spacer further enhanced spin-to-charge conversion by 1.7 times. Lastly, (110)-oriented $RuO_2$ grown on MgO, demonstrated low spin memory loss (15%) and high spin transparency (90%). These results establish $MoS_2$, $Bi_2Se_3$, and $RuO_2$ as promising candidates for next-generation spintronic devices, offering efficient spin dynamics and enhanced performance. We have tried to understand the spin pumping phenomena and have quantified the important spintronic parameters relevant for future spintronic applications.

**t0009**

**Investigation of Physical Properties of Frustrated Ternary Oxides**

Jogendra Kumar

*School of Physical Sciences, Indian Institute of Technology Mandi, Mandi, 175075, Himachal Pradesh, India*

*Email: jogendrak262@gmail.com*

Frustrated rare-earth magnets are of great interest due to their ability to host exotic magnetic ground states such as spin ice and spin liquid. This thesis investigates the rare-earth-based ternary oxides $R(Ta,Nb)O_4$ as a platform for exploring such phenomena. $GdTaO_4$, $GdNbO_4$ and $DyNbO_4$ compounds exhibit enhanced cryogenic magnetocaloric effects near the liquid helium regime, driven by short-range magnetic correlations. $TbTaO_4$ and $DyTaO_4$ show thermally activated spin relaxation associated with crystal electric field excitations. In Nd-based compounds, bulk measurements and DFT calculations confirm the development of an effective spin-½ ground state. Combined bulk and muon spin relaxation studies reveal a correlated dynamical ground state in $YbNbO_4$, while $YbTaO_4$ stabilizes a spin–orbit-entangled $J_{eff}$ = ½ state in a quasi-two-dimensional lattice. These findings highlight the rich interplay of spin-orbit coupling, crystal electric field effects, magnetic frustration, and dimensionality in shaping unconventional magnetism.

**t0010**

**Novel magnetic ground states, electrical transport properties and their relationship with chemical order in Heusler alloys**

Koushik P*

*School of Physical Sciences, Indian Institute of Technology Mandi, Mandi 175075, Himachal Pradesh, India* *

*Email: koushikprao1@gmail.com*

Heusler alloys are a versatile material class with immense potential for applications based on novel quantum phenomena like topological states and half-metallic ferromagnetism. However, their promising properties are often undermined by the unavoidable presence of structural and chemical disorder during synthesis. Employing a comprehensive approach that combines targeted

material synthesis with detailed structural, magnetic, and electrical transport characterization, this work establishes that disorder is not merely a defect but a powerful tuning parameter. My findings reveal that varying degrees of atomic disorder can drive these materials into exotic magnetic ground states, including cluster glass, re-entrant glass, and a novel "partially disordered" phase where glassy dynamics and long-range antiferromagnetism coexist. Crucially, this research uncovers the deep influence of disorder on electronic transport, highlighted by an unconventional scaling relationship in the anomalous Hall effect in Ir-Mn-Sn, which challenges existing theories. A comparative study between $Pd_2TbSn$ and $Pd_2HoSn$ provides a clear, controlled demonstration of how disorder can completely transform a material's magnetic character. Collectively, this work provides fundamental insights into the physics of disordered materials. It underscores that understanding and controlling the structure-property relationship is critical to intentionally engineering Heusler alloys and unlocking their full technological potential.

**t0011**

**Atomistic Models of IPG – Development, Structural Characterisation and Properties Through Simulation**

Shakti Singh[1,2,3]
[1] *Photonic Materials Technology Section, RRCAT, Indore, Madhya Pradesh 452013 India*
[2] *(Erstwhile) MSG, IGCAR, Kalpakkam, Tamilnadu 603102 India*
[3] *Homi Bhabha National Institute (HBNI), Mumbai, Maharashtra 400094 India*
**Email: shaktis@rrcat.gov.in*

Structure of glasses is nearly a century-old research topic. The thesis adopts an altogether different approach of modelling glasses wherein the models are obtained using force-relaxation of random-network models generated through a potential-free Monte-Carlo (MC) method-based approach rather than the conventional route of melt-quench simulations. The material of interest here is iron phosphate glass (IPG), whose most popular use is in radioactive waste immobilization. But modelling even simple glass like silica is a non-trivial task owing to presence of disorder and absence of long-range order. The thesis presents random-network modelling of initial configurations of glasses using the MC method, employing the available structural knowledge from experiments and post-processed using DFT or CMD. Using DFT, the electronic structure of IPG is accurately predicted with properties like band-gap, vibrational density of states and elastic constants agreeing closely with experiments. The CMD based study models the medium-range (MR) structure of IPG validated using rings distribution and structure factor comparison. It also compares IPG models produced using various randomization routes. Finally, the composition-property correlation is studied by generating models of different composition using MC method, post-processed using DFT, which corroborates various trends observed experimentally.

**t0012**

**High Pressure Magnetic, Transport and Spectroscopic Investigations on some Cu based Insulators and Layered Metallic Systems**

*Subodha Sahoo[1, 2a)]*
[1]*HP & SRPD, Bhabha Atomic Research Centre, Mumbai, 400085, India*
[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*
[a)] *Email: subodhas@barc.gov.in*

Material investigations have long played a vital role in advancing human civilization. Exploring materials under extreme conditions, such as high pressure, low temperature, and magnetic field- reveals a range of novel phenomena, including superconductivity, charge density waves, insulator-to-metal transitions, structural transformations, and magnetic ordering. The present thesis investigates the impact of pressure on two categories of materials, copper-based insulators ($CuB_2O_4$, $Cu_2OSeO_3$ and $ZnCu_3(OH)_6Cl_2$) and novel layered metallic systems ($VSe_2$, $PdCoO_2$, and (Fe, S) co-doped $Bi_2Se_3$). Various experimental techniques viz., synchrotron based XRD, optical absorption, electrical resistance, magneto-transport and SQUID based magnetization have been carried out to study the pressure effect on the structure-property relationships. Significant outcomes include the discovery of a pressure-induced structural phase transition and the construction of a P-T-H phase diagram in $CuB_2O_4$; the pressure-driven melting of the quantum spin liquid state in Herbertsmithite; and in $VSe_2$, the pressure induced enhancement of charge density wave ordering to room temperature from ~110 K and the emergence of superconductivity associated with a structural transition.

**t0013**

**Exploring the Magnetic Excitations of Trimer Ruthenates using Inelastic Neutron Scattering and Machine Learned Force Field Calculation**

E. Kushwaha,[1] M. B. Stone,[2] and T. Basu[1, a)]
[1]Rajiv Gandhi Institute of Petroleum Technology, Jais, Amethi, 229304, India
[2]Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA
[a)] *Email: tathamay.basu@rgipt.ac.in*

We have performed the Inelastic Neutron Scattering (INS) experiment on the trimer-based ruthenate $Ba_5Ru_3O_{12}$ system. Unlike other trimer ruthenates that typically adopt collinear or non-magnetic configurations, this system exhibits long-range antiferromagnetic order below $T_N$, which is 60 K with a non-collinear spin arrangement. This unconventional magnetism arises from geometric frustration, strong spin-orbit coupling (SOC), and competing intra-trimer exchange interactions among three inequivalent Ru sites. INS measurements reveal two spin-wave excitations: one less intense excitation around 5.6 meV and another broad intense excitation around 10-15 meV. Above $T_N$ a single broad excitation is observed around 6-16 meV,

indicating short-range spin correlations in the paramagnetic phase. We have also performed SpinW simulations to reproduce the observed spectra. Also, additional intensity is observed at high momentum transfer (Q) and in the same energy range which suggests possible spin-phonon coupling. We predict the ground state of $Ru_3O_{12}$-isolated trimer through theoretical calculations which agree with the experimentally observed spin excitation. We have also performed Phonon calculations through Machine Learned Force Field (MLFFs) calculation which confirm minimal overlap with magnetic scattering in the relevant Q-range and validate the observed excitations through INS simulations.

**t0014**

**The Micro-scale structuring as a route to modification in mechanical properties of biopolymer composites and hydrogels for biomedical applications**

Tithi Joshi and Debjani Bagchi
*Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara 390002, Gujarat, India.*
*Email: tithijoshi8@gmail.com*

Although hydrogels with a huge number of chemical compositions have been developed by several groups, the mechanism of their activity at micro and nanoscale has not been investigated and correlated to macro scale properties. This thesis aims to bridge this gap. Cross-linked starch films with citrate ions and glycerol or sorbitol as plasticizers demonstrated superior mechanical properties, including higher Young's modulus and tensile strength. A biocatalyst was used to improve the cross-linking efficiency and stiffness. Incorporation of nanoparticles like bentonite and carboxymethyl cellulose (CMC) enhanced flexibility but reduced tensile strength and modulus. CMC offered the best mechanical performance overall, despite causing microcrack formation and non-linear elasticity. Nanoindentation revealed the spatial heterogeneities in film stiffness and modulus, and it was observed that nanoparticles reduced creep and enhanced stiffness. Small angle X-ray Scattering (SAXS) and fluorescence probe diffusion assays reveal that nanoparticle concentration influences pore structure and drug diffusion. The results highlight how mechanical and structural properties work together to optimize drug delivery and bioactivity.

**t0015**

**Order-Disorder Phase Transition in Pyrochlore Oxides under Pressure, Irradiation, and Temperature**

[1, a] Yogendar Singh, [1]Pawan Kumar Kulriya
[a]*Email: yogendarsingh7878@gmail.com*

This thesis is focused on the essential findings and explanations of the thesis, along with an outlook for future research into pyrochlore oxides in nuclear industry applications. In this thesis, bulk $GdYTi_2O_7$, $Nd_2Zr_2O_7$, $Nd_{1.8}Zr_{2.2}O_{7.1}$, $Gd_2Ti_{2-y}Zr_yO_7$, nc-$Gd_2Ti_2O_7$, and nanocrystalline high entropy $(La_{0.2}Nd_{0.2}Sm_{0.2}Gd_{0.2}Yb_{0.2})_2Zr_2O_7$ were chosen as prime candidates to study the behavior of pyrochlores under extreme conditions and thermal conductivity at elevated temperatures. The high-pressure structural stability of conventional and high-entropy pyrochlores is discussed in detail. This thesis also examines the local structure modifications in swift heavy irradiated pyrochlores using synchrotron (XAS) experiments to explore the stability under ion irradiation. In addition, we have investigated how stoichiometry and composition affect phase recovery in ion-irradiated pyrochlores. The thesis outcomes have demonstrated that the disordering of the polyhedron, the cationic radius ratio, stoichiometry, and compositions of the pyrochlore-type oxides all play a significant role in modulating the structural properties under extreme conditions.

**t0017**

**Non-Collinear Spin-Induced Magnetic and Magnetotransport Phenomena in Intermetallic Compounds**

Afsar Ahmed[1, a)] and Indranil Das[1]
[1] *Saha Institute of Nuclear Physics, A CI of HBNI, 1/AF Bidhannagar, Kolkata 700064, India*
[a)]*Email: afsarsci@gmail.com*

The interplay between topology and magnetism in quantum materials has led to the discovery of unconventional transport phenomena such as the topological Hall effect (THE) and the unconventional anomalous Hall effect (UAHE). These effects originate from real-space non-collinear spin textures and momentum-space topological features like Weyl points, respectively. However, realizing both topologies in a single system remains a challenge due to contrasting symmetry requirements. This thesis explores intermetallic compounds—particularly inverse Heusler alloys, β-Mn, and hexagonal magnets—as promising platforms to co-stabilize these topological phases, offering insights into emergent electrodynamic responses and advancing next-generation spintronics applications.

**t0018**

**Aspects of Electronic Band Topology and Superconductivity in Transition Metal Dichalcogenides**

M. Singh and S. Patnaik
*School of Physical Sciences, Jawaharlal Nehru University, New Delhi 110067, India)*
** Email: spatnaik@mail.jnu.ac.in*

The relationship between superconductivity and topology in transition metal dichalcogenides (TMDs) is examined in this thesis, with particular attention on $SnTaS_2$, $Sn_{0.5}Ta_{0.5}S_2$, and Cu-doped TiSeS. The study demonstrates the successful tuning of superconducting and normal-state properties by the use of elemental substitution, intercalation, and controlled disorder. This work reveals signatures of topologically non-trivial superconducting states and emphasizes the struggle between superconductivity and

charge density wave order. These discoveries shed more light on the processes underlying unusual superconductivity in layered materials.

**t0019**

**First Principles Studies of Post Transition Metal based Janus Layers for the Water splitting Hydrogen production**

Anjana E Sudheer[1] and D Murali[1,a)]
*[1]Indian Institute of Information Technology Design and Manufacturing Kurnool Andhra Pradesh Kurnool, 518007*
*[a)]Email: dmurali@iiitk.ac.in*

Solar-assisted photocatalytic water-splitting is one of the sustainable ways to produce hydrogen. Herein, we design novel Janus layers PbXY (X, Y = F, Cl, Br, I), SnIX (X=Br/Cl) and SbXY (X=Se, Te, Y=I, Br) using the Density Functional Theory (DFT) calculations. We assure the energetic, vibrational and thermal stability of the Janus layers and propose experimental conditions required for synthesis with help of phase diagram. The electronic and optical properties shows that the designed JLs posess superior charge transfer and optical properties. The band alignment obtained from the GW result shows all the JLs have band alignment that straddle water redox potential at acidic condition. The Gibbs free energy analysis also shows that the HER and OER reactions are possible in light on condition with the help of additional energy 1-1.5 eV in all the material. Finally, we shows that the strain engineering can drastically reduce the additional energy required for the HER and OER reactions in the JLs.

**t0020**

**Investigations of Broadband Dielectric Response and Other Properties of Some Complex Perovskite-Based Materials**

Nitin Kumar[1,a], K Sandeep Rao[2,3], S. N. Achary[2,3], S.K. Deshpande[1]
*[1]UGC-DAE Consortium for Scientific Research Mumbai Centre, Bhabha Atomic Research Centre, Mumbai, 400085, India*
*[2]Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India*
*[3]Chemistry Division, Bhabha Atomic Research Centre, Mumbai, 400085, India*
**Email: nk50194@gmail.com*

Energy plays a vital role in human life and national economic development. With growing global population and industrialization, energy demand is increasing rapidly. Currently, most energy needs are met using non-renewable sources such as coal, petroleum, and natural gas, which are depleting and environmentally harmful. Hence, there is an urgent need for clean, renewable alternatives for both energy generation and storage. Solid oxide fuel cells (SOFCs) are a promising clean energy technology, but their high operating temperatures (>700°C) cause durability and cost issues. Research is focused on developing electrolytes with high ionic conductivity and stability at moderate temperatures (300–600°C). Similarly, energy storage devices require efficient dielectric materials with high permittivity and low dielectric loss for miniaturized electronics and wireless communication. Perovskite-type oxides (ABO3) are promising materials due to their structural flexibility and wide range of properties, from insulating to conducting, and paramagnetic to ferromagnetic behavior. Their structure can be tuned via ionic size, defects, or octahedral connectivity. Transition metal-containing perovskites, especially double perovskites (Ln2M′M″O6), offer tunable electrical and magnetic properties. Hexagonal perovskite derivatives such as Ba3MM′O8.5 (M = W, Mo; M′ = Nb, V) exhibit high oxide ion conductivity at moderate temperatures, making them promising candidates for next-generation energy applications.

**t0021**

**Studies of Epitaxial Adlayers on Monocrystalline Substrates Using Scanning Tunnelling Microscopy and Related Techniques**

Pramod Bhakuni
*UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore, 452001, Madhya Pradesh, India*
**Email: bhakuni.pramod188@gmail.com*

We present a comprehensive investigation of the surface and electronic properties of epitaxially grown Ga and Sn adlayers on various monocrystalline substrates using surface-sensitive techniques. Our work explores how the surface structure and electronic properties of these adlayers are modified across diverse range of substrates: 3*d* metals [Cu(111) and Ni(111)], a ternary quasicrystal [icosahedral (*i*)-Al-Pd-Mn], a magnetic topological insulator (Sb-doped $MnBi_2Te_4$), and a Heusler alloy [$Ni_2MnGa$(100)]. Ga films grown on Cu(111) exhibit various reconstructions, possibly due to Cu-Ga alloying; while on *i*-Al-Pd-Mn, Ga adopts a quasicrystalline form with distinct quasiperiodic motifs. We demonstrate the formation of multilayer stanene on Ni(111), which shows a nearly planar honeycomb with a $p(2\times2)$ structure and a buckled honeycomb with (1×1) structure on MBST, both facilitated by an alloyed buffer layer. Additionally, $c(4\times2)$ and $(\sqrt{3}\times\sqrt{7})R30°$ phases were identified with low temperature Sn deposition on Ni(111). On $Ni_2MnGa$(100), an ordered $\beta$-Sn film is formed after annealing. Studies on $LaTe_3$ and $YTe_3$ reveal an incommensurate unidirectional charge density wave, with the latter exhibiting the formation of twin domains that are orthogonal to each other.

**t0022**

**Ferromagnetic Resonance Study Of Magnetic Oxides For Their Spintronic Applications**

Kishori Lal
*Department of Physics, Indian Institute of Technology Kanpur, Kanpur 208016, India*
**Email: kishori@iitk.ac.in*

Ferromagnetic resonance (FMR) spectroscopy is a vital tool for exploring magnetization dynamics in spintronic materials. In this thesis, we investigate rare-earth iron garnets (REIGs), namely $Bi_3Fe_5O_{12}$ (BIG) and $Yb_3Fe_5O_{12}$ (YbIG), as well as $La_{0.7}Sr_{0.3}MnO_3$ (LSMO)-based oxide heterostructures, for their magnetic anisotropy and damping properties. Perpendicular magnetic anisotropy (PMA) was achieved in sub-10 nm thick BIG and YbIG films grown epitaxially on $Gd_3Ga_5O_{12}$(111) substrate, attributed to strain-induced magnetoelastic and magnetocrystalline anisotropies enhanced by high spin-orbit coupling ions ($Bi^{3+}$, $Yb^{3+}$). For the BIG films, a reorientation of the easy axis from oblique to out-of-plane was observed as thickness reduced from 15 nm to 10 nm. Thickness variation in YbIG films showed tunable PMA and sixfold symmetry in IP FMR, with damping factors ~$10^{-2}$. Further, we probed Rashba SOC-driven magnetization dynamics in LSMO/$LaTiO_3$(δ)/$SrTiO_3$ heterostructures. The increasing LTO thickness (0–12 u.c.) modifies the 2DEG properties and enhances damping, IP anisotropy, and effective magnetic fields, establishing tunability of magnetic response via interface engineering. Our results demonstrate the potential of magnetic oxides and engineered interfaces for energy-efficient spintronic and magnonic devices.

**t0023**

**Structure-Luminescence Correlation Studies in $Eu^{3+}$ Doped Calcium Magnesium Silicate Phosphor**

Navya Sara Kuriyan[1, a)], P. S. Ghosh[2], Aiswaria Deepti[3], M. Parvathy[1], A. K. Arya[2], P. S. Baby Chakrapani[3] and M. Sabeena[1]
[1]*Department of Physics, Cochin University of Science and Technology, Kochi- 682022, Kerala, India.*
[2]*Glass and Advanced Materials Division, Bhabha Atomic Research Centre, Trombay, Mumbai- 400085, India.*
[3]*Center for Neuroscience, Department of Biotechnology, Cochin University of Science and Technology, Kochi- 682022, Kerala, India.*
**Email: navyasarakuriyan@cusat.ac.in (Email of corresponding author)*

This study investigates how crystal structure modifications influence the photoluminescence (PL) properties of $Eu^{3+}$ doped calcium magnesium silicate (CMS: $Eu^{3+}$) phosphors, using both experimental and theoretical approaches. CMS: $Eu^{3+}$ exists predominantly in four crystalline phases: diopside ($CaMgSi_2O_6$) and merwinite ($Ca_3MgSi_2O_8$) of monoclinic crystal structure, akermanite ($Ca_2MgSi_2O_7$) of tetragonal crystal structure and monticellite ($CaMgSiO_4$) of orthorhombic crystal structure. By varying the synthesis methods, the phases of CMS: $Eu^{3+}$ were optimized to enhance the PL properties and thereby the suitability for biomedical applications, such as in vitro bioimaging and tissue scaffolding. Among the studied phases, diopside is obtained as the most efficient host for $Eu^{3+}$, demonstrating significant potential for in vitro bioimaging.

**t0024**

**Study of Optical Properties of Some Binary Semiconductors Using Linear Response Theory**

Nikhil Joshi*
*Department of Physics, Mohanlal Sukhadia University, Udaipur-313001, India*
**Email: phd22_nikhil@mlsu.ac.in*

In determining the optical properties of semiconductors, the excitons [i.e. electron-hole (*e-h*) interaction], play important role. The linear response time dependent density functional theory (TD-DFT) is an efficient tool which incorporates *e-h* interaction through appropriate exchange-correlation (XC) kernel. Two such kernels which takes excitonic effect into account are long range corrected (LRC) and bootstrap (BS) kernels. In this work, the linear response TD-DFT with LRC and BS kernels are used to obtain optical properties and electron energy loss spectra (EELS) of binary compound semiconductors BAs, ZnS and ZnSe. Additionally, adiabatic local density approximation (ALDA) and random phase approximation (RPA) are also used for comparison purpose. In addition we have examined the impact of the local field effect (LFE) on the optical and EEL spectra. Furthermore, an alternative approach based on the pseudopotential form factors (FFs) employed in the empirical pseudopotential method is developed and utilized to find the material dependent parameter $\alpha$ required in the LRC kernel. The method has been proved to be novel and is found to work well for the zincblende (zb) semiconductors. A systematic investigation of effect of various values of $\alpha$ on optical and EEL spectra is presented. It is noted that the better choice of this parameter leads to more accurate optical spectra.

**t0026**

**Emergent Transport and Magnetic Behavior in Oxide Thin Films and Heterostructures: Unveiling the Role of Interface Engineering and Spin-Orbit Coupling**

A.G. A. Rahman and A. K. Pramanik
*School of Physical Sciences, Jawaharlal Nehru University, New Delhi-110067, India*
**Email: arifa.rahman13@gmail.com*

Here, we report a comprehensive investigation of interface-driven magnetic and transport phenomena in epitaxial oxide heterostructures. This work involves four distinct investigations, involving different oxide materials of timely interests. Focusing on $La_{0.67}Sr_{0.33}MnO_3/Pr_2Ir_2O_7$ (LSMO/PIO) and $La_{0.67}Ca_{0.33}MnO_3/SrIrO_3$ (LCMO/SIO) bilayers, our works uncover how spin-orbit coupling (SOC) at 3d-5d oxide interfaces profoundly modifies the ground-state properties. In the LSMO/PIO bilayer, interfacial Dzyaloshinskii-Moriya interaction (DMI) modifies the magnetic structure, giving rise to weak localization effect in electronic charge transport. The LCMO/SIO bilayer exhibits a temperature-driven crossover in magnetoresistance (MR), that essentially evolves to an asymmetric positive MR at low temperature due to SOC-mediated interfacial scattering. We have further studied current-voltage (I-V) characteristics and resistive switching in substrate dependent $La_{0.67}Sr_{0.33}MnO_3/SrMnO_3$ / $La_{0.67}Sr_{0.33}MnO_3$ trilayers. In the last chapter, synthetic antiferromagnetic coupling has been studied in $Pr_{0.6}Sr_{0.4}MnO_3$ /$CaRuO_3$/ $Pr_{0.6}Sr_{0.4}MnO_3$

multilayers, which has been tuned through modification in both magnetic and spacer layer thickness. These results highlight the potential of interface engineering in designing oxide heterostructures for future spintronic applications.

**t0027**

**Observation of Martensite Phase Transformation and Positive Magnetoresistance in Off-Stoichiometric $Co_2Fe_{0.5}Ti_{0.5}Si$ Thin Films**

*Mainur Rahaman[1], Lanuakum A Longchar[1], Rajeev Joshi[2], R. Rawat[2], M. Manivel Raja[3], S. N. Kaul[1], and S. Srinath[1, *]*
*[1] School of Physics, University of Hyderabad, Hyderabad-500046, Telangana, India*
*[2] UGC - DAE Consortium for Scientific Research, Indore-452001, India*
*[3] Defence Metallurgical Research Laboratory, Hyderabad-500058, Telangana, India*
** Email: srinath@uohyd.ac.in*

This work investigates the structural and transport properties in off-stoichiometric $Co_2Fe_{0.5}Ti_{0.5}Si$ (CFTS) Heusler alloy thin films with two different thicknesses, t = 15 nm and 35 nm, deposited on Si(100) substrate at a substrate temperature (TS) of 500 °C by ultrahigh vacuum magnetron sputtering technique. Both the CFTS films show B2 crystalline order. Temperature-dependent resistivity measurements reveal a distinct thermal hysteresis and sudden drop in resistivity near 250 K, indicative of a thermo-elastic martensitic phase transformation (MPT). In the martensite phase, both films show a very small negative temperature coefficient of resistivity (n-TCR), and the corresponding conductivity is well described by a spin gapless semiconductor (SGS)-based two-channel model. Transverse magnetoresistance remains weak (< 1%) in the martensitic phase but increases sharply near 250 K, reaching a maximum of ∼ 12% at 325 K.

**t0029**

**Optimization and Characterizations of Oxide Based Thin Film Devices**

Bharavi Hirpara
*Department of Physics, Saurashtra University, Rajkot - 360005*
**Email: bahirpara7@gmail.com, bahirpara@sauuni.ac.in*

High resistive magnetic oxides that can be used for energy storage applications, memory materials, sensors, and neuromorphic components of artificial intelligence are needed in today's materials quest. In light of these potential requirements for high resistive magnetic materials, the current thesis has examined low doped p-type mixed valent manganites, delving further into $Y_{0.9}A_{0.1}MnO_3$ (A = Ca & Sr) systems and $La_{0.9}Sr_{0.1}MnO_3$ thin film devices. Since the influence of the shape of the manganite systems is intriguing and worthwhile to comprehend, polycrystalline bulk, thin film devices, and multilayers have been taken into consideration for Y-based manganites in the current thesis. Correlations between structure and physical properties have been developed for better feasible designs and uses of these materials, and a variety of experimental characterizations have been carried out to understand the structure of all these systems.

**t0030**

**Study of Lumino-Structural Properties of Rare Earth Ions Doped Niobate Phosphors for Opto-Electronic Applications**

Kanishk Poria[1,*], Nisha Deopa[2] and Jangvir Singh Shahi[1]
[1]*Department of Physics, Panjab University, Chandigarh.*
[2]*Department of Physics, Chaudhary Ranbir Singh University, Jind.*
**Email: kanishk.chaudhary15@gmail.com*

This thesis reports the development and detailed investigation of a novel phosphor material based on $Dy^{3+}$ and $Eu^{3+}$ doping for advanced solid-state lighting applications, particularly white LEDs. $Dy^{3+}$ and $Eu^{3+}$ activated $Na_3Ba_2LaNb_{10}O_{30}$ phosphors were synthesized via the solid-state reaction method, chosen for its scalability and ability to produce phase-pure, thermally stable materials. Structural and morphological analyses using XRD, FESEM, Raman, FTIR, and EDS confirmed the successful incorporation of dopant ions without distortion of the host lattice. Photoluminescence studies revealed that $Dy^{3+}$-doped samples emitted blue and yellow light suitable for white light generation, while $Eu^{3+}$-doped phosphors exhibited strong red emission due to the $^5D_0 \rightarrow {}^7F_2$ transition. The optimized doping concentrations were 7 mol% for $Dy^{3+}$ and 9 mol% for $Eu^{3+}$, beyond which luminescence was quenched. Time-resolved measurements confirmed long-lived emission (300 µs for $Dy^{3+}$, 800 µs for $Eu^{3+}$), while internal quantum yields reached 45% and 78% respectively, indicating strong commercial viability. These findings are significant for advancing sustainable, energy-efficient lighting and pave the way for integrating these materials into next-generation optoelectronic devices.

**t0032**

**Large Area Fabrication of Two-Dimensional $PtX_2$ (X=S, Se) Heterostructures For Broadband Photodetector Studies**

Gaurav Bassi and Mukesh Kumar
*Functional and Renewable Energy Materials Laboratory, Department of Physics, Indian Institute of Technology Ropar, Rupnagar, Punjab-140001, India*
*Email: gaurav.19phz0005@iitrpr.ac.in*

Photodetectors are optoelectronic devices that convert light signals into electrical signals and are used to detect a range of the electromagnetic spectrum. My thesis aims to develop $PtX_2$ (X=S, Se) heterostructure-based broadband photodetectors with high performance in the near-infrared (NIR) region. Broadband photodetectors have multiple applications in optical communication,

defense security, environmental monitoring, and medical imaging. Two-dimensional (2D) materials, especially group-10 transition metal dichalcogenides (TMDC), $PtX_2$ are highlighted for their distinct properties including narrow band gap range, high carrier mobility, and good ambient stability, required to fabricate high-performance broadband photodetectors. The thesis achieved multiple goals including the large area and controlled growth of $PtS_2$ film by thermally assisted conversion (TAC) method where pre coated Pt film are sulfurized in chemical vapor deposition (CVD). The various growth parameters such as sulfur amount, Pt thickness and carrier gas flow rate are optimized to achieved the high quality $PtS_2$ film on different substrates ($SiO_2$/Si, Si, sapphire and mica). Next, various $PtX_2$ heterostructures including $PtS_2/MoS_2$ (2D-2D), $PtS_{2-x}/Ga_2O_3$ (2D-3D) and $PtSe_2/MoS_2$ based broadband photodetectors with best response in the NIR region are fabricated. Moreover, using X-ray photoelectron spectroscopy (XPS) detailed interface study of the heterojunction including their band alignment and carrier transport mechanism is also carried out. Therefore, this work may help to grown large area growth of $PtX_2$ and their heterostructure for future optoelectronics applications.

**t0033**

**Band Topology & Role of Electronic Structure on Transport Properties of Nonsymmorphic Single Crystals**

Suman Nandi and Arumugam Thamizhavel
*Department of Condensed Matter Physics and Materials Science,*
*Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai 400005, India*
** Email: suman.nandi121998@gmail.com*

My research focuses on the role of the electronic structure in governing the transport properties of a series of nonsymmorphic transition metal pnictides and stannides: $ZrAs_2$, $ZrSn_2$, $CoSn_2$, and $HoSn_2$. The progression from Zr-based compounds ($ZrAs_2$ and $ZrSn_2$) to those containing Co ($CoSn_2$) and Ho ($HoSn_2$) introduces increasingly localized and strongly interacting electrons. Zr, with its 4*d* orbitals, contributes relatively delocalized electronic states with weak electron-electron interactions, resulting in well-dispersed bands and metallic behavior. In contrast, 3*d* electrons in Co are more localized, enhancing Coulomb interactions, and correlation effects. This feature can enhance electronic instabilities and significantly affect transport behavior. Further in $HoSn_2$, the addition of highly localized 4*f* electrons from Ho ions induces long range magnetic ordering. Their coupling to conduction electrons can generate a variety of intriguing transport behaviors.

**t0034**

**Investigation of Spin-Phonon coupling, Magnetic and Magnetocaloric properties in Al substituted Multiferroic $GaFeO_3$**

Saarthak Dulgaj[a], Anshu Gaur[a], Vasanth Sathe[b], P D Babu[c], S. N. Kaul[a] and S. Srinath[a *]
[a] *School of Physics, University of Hyderabad, Telangana, 500046, India*
[b] *UGC - DAE Consortium for Scientific Research, Indore 452001, India*
[c] *UGC DAE Consortium for Scientific Research, BARC, Mumbai 400085, India*
** Email: srinath@uohyd.ac.in*

Al-substituted orthoferrite $GaFeO_3$ is a promising room-temperature multiferroic material [1-3]. In addition to their multiferroic properties, these materials are also interesting for exploring magnetocaloric and spin-phonon coupling (SPC) effects. This study offers a comprehensive investigation of the structural, magnetic, magnetocaloric, and SPC properties of $Ga_{0.7}Al_{0.3}FeO_3$ (GAFO), synthesized via the sol-gel method [2-4]. Rietveld refinement of the X-ray diffraction data confirms a single-phase orthorhombic $Pc2_1n$ structure with an average crystallite size of approximately 63 nm. Magnetic measurements showed an increased Néel temperature ($T_N \approx 240$ K) compared to $GaFeO_3$. Magnetocaloric effect (MCE) analysis, based on isothermal magnetization data, revealed a peak magnetic entropy change ($-\Delta S_M$) near $T_N$ and refrigerant capacity consistent with mean-field critical behaviour. Raman spectroscopy from 100-300 K reveals 27 active modes, 10 of which show temperature-dependent behaviour. By fitting the entire temperature range with anharmonic and SPC terms, the SPC constant ($\lambda$) is identified into groups of modes based on coupling strength into weak, intermediate, and strong, corresponding to librational, symmetric, and asymmetric polyhedral vibrations, respectively. These results show a relationship between the vibrational mode symmetry and spin-lattice interaction strength, establishing GAFO as a multifunctional material.

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**t0037**

**Advanced Studies on the Thermoelectric Properties of $Cu_2Se$ Based Nanostructures**

Parvathy T[1, a)] and P.P.Pradyumnan[1]
[1]*Department of Physics, University of Calicut, Malappuram-673635,Kerala,*
[a)]*Email: parvathysivadass@gmail.com*

Thermoelectric materials have gained significant attention in recent years due to their potential to address key challenges in energy conversion and waste heat recovery. However, its practical implementation is hindered by challenges such as high material costs, limited operational temperature ranges, and difficulty of simultaneously optimizing electrical and thermal transport properties. Among these materials, $Cu_2Se$ has emerged as a promising p-type semiconductor due to its unique phonon-liquid electron-crystal behavior. This thesis focuses on enhancing the thermoelectric performance of $Cu_2Se$ through systematic material engineering strategies including doping, dual doping, and nanoinclusion approaches. Ni doping induces band sharpening, optimizing carrier effective mass and increasing carrier mobility. Building on this, co-doping with Ni and Zn introduces additional lattice distortions, intensifying phonon scattering and improving thermoelectric efficiency. Furthermore, the incorporation of ZnSe nanoinclusions via planetary ball milling facilitates band convergence and enhances carrier transport. MgO nanoinclusions contribute by inducing energy filtering effects and strong phonon scattering at heterointerfaces. The combined effects of these strategies resulted in a remarkable enhancement of thermoelectric performance, with several compositions exhibiting a dimensionless figure of merit (ZT) exceeding 1. The findings offer valuable insights into developing efficient, low-cost thermoelectric materials for future waste heat recovery and sustainable energy applications.

**t0038**

**Topological Phase Transition in Some Selected Materials: A First-Principles Study**

Ramesh Kumar[1,a] and Mukhtiyar Singh[1]
*[1]Computational Quantum Material Design (CQMD) Lab, Department of Applied Physics, Delhi Technological University, Delhi-110042, India*
*[a)] Email: rk.bishnoi1995@gmail.com*

In this work, we present the evolution of the topological phase in the materials of rare-earth monopnictides, Zintl, and chalcogenides families with hydrostatic pressure or epitaxial strain. These materials have a stable, topologically trivial semimetallic nature at ambient pressure. First, we have identified the actual ground states of these system with an appropriate choice of exchange-correlation functionals. Furthermore, we have analysed the structural stabilities of these materials with applied pressure or strain using the phonon dispersion spectrum. The topological phase transition under the applied hydrostatic pressure and epitaxial strain has been observed with the inverted contribution of the orbitals in the bulk band inversion, and the same has been confirmed with the presence of topological surface states in the surface density of states. The $Z_2$ topological invariants and Chern number have been calculated using parity analysis of all the occupied bands and Wannier charge centers (WCCs). This study of various systems can be further used as a reference for experimental analysis of topological phases in these materials.

**t0040**

**Berry phase effects in the transport properties of intermetallic single crystals**

Gourav Dwari [a)] and Arumugam Thamizhavel
*Department of Condensed Matter Physics and Materials Science,*
*Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai 400005, India*
*[a)]Email: gouravdwari1@gmail.com*

Discovering new materials with exotic phases and intriguing properties has always been an exciting task among the materials science research community as they provide an ideal ground to explore the fundamental areas of physics while sometime, they are proved to be exceptional for some novel applications. In this thesis, we present the investigation of the anisotropic physical properties, Fermi surface studies and Hall response of a few selected intermetallic compounds in bulk single crystalline form. Hall effect arises because of the Lorentz force experienced by the charge carriers in materials. Magnetism and electronic band structure play important roles in this case. Generally, in non-magnetic compounds, this Lorentz force experienced by the charge carriers is due to the external magnetic field that results in the ordinary Hall effect (OHE). The response of such materials can be linear or non-linear with applied magnetic field depending on whether it is a single band or multiband system. In terms of an application point of view, semiconducting materials with linear Hall response are extensively used as Hall sensors. On the other hand, in ferromagnets, total gauge field in the momentum space, also known as the Berry curvature, causes the charge carriers to pick up an additional anomalous velocity perpendicular to the electric field, resulting in the anomalous Hall effect (AHE). Similarly, a Berry curvature originating from real space can deflect the conduction electrons and topological Hall effect (THE) can be realized. We have studied the thermodynamics and magnetotransport behaviors of single crystals exhibiting different types of Hall responses and presented the results here.

**t0042**

**Defect Engineering via Aliovalent Doping for Enhanced Scintillation Performance in Halide Single Crystals**

Durgesh Singh Sisodiya
*Homi Bhabha National Institute, Mumbai, India*
*Bhabha Atomic Research Centre, Mumbai, India*
**Email: dsinghsisodiya1996@gmail.com*

Inorganic halide scintillators such as CsI:Tl and $CeBr_3$ are widely used in high-energy physics, medical imaging, security screening, and neutron detection. However, CsI:Tl suffers from afterglow, while $CeBr_3$ exhibits high hygroscopicity and poor mechanical properties, limiting their performance and large-scale deployment. In this work, an aliovalent doping and co-doping approach was employed to address these challenges. Density functional theory (DFT) calculations on CsI:Tl doped with $Sr^{2+}$ and $Eu^{2+}$ revealed the formation of deep trap centers that suppress afterglow by capturing charge carriers, which was experimentally validated through thermoluminescence measurements. For $CeBr_3$, aliovalent dopants ($Ca^{2+}$, $Sr^{2+}$, $Ba^{2+}$) were systematically investigated for their influence on crystal growth, hygroscopicity, and scintillation performance. $Ca^{2+}$ doping improved energy resolution (4.7% to 4.3% at 662 keV), while $Ba^{2+}$ doping significantly reduced hygroscopicity (~26%) and enhanced growth yield. The improvements in energy resolution were attributed to $Br^-$ vacancy defects introduced to maintain charge neutrality upon aliovalent doping. A double-doping strategy combining $Ca^{2+}$ and $Ba^{2+}$ yielded up to ~25% higher light yield and improved energy resolution (4.1% at 662 keV) compared to undoped $CeBr_3$. These findings demonstrate that aliovalent doping and co-doping are effective tools for tailoring defect structures in halide scintillators, enabling simultaneous enhancement of scintillation performance, crystal growth, and environmental stability.

**t0044**

**Synthesis, Instrumentation and Studies of Charge and Magnetic Ordering Phenomena in Certain Nano Manganites**

Pratheek
*IIT Bombay, Mumbai*
*pratheek245@gmail.com*

Charge ordering (CO) suppression in manganites is studied extensively by several groups but still it's an un settled issue. There is evidence of disappearance of charge order on reduction of size of the particle. However, the synthesis method adopted by various groups is either sol gel or combustion methods where one does not have satisfactory control over the size of the particles synthesized. This motivated us to adopt Reverse Micelle method of synthesis of nano particles where the size can be controlled by the appropriate selection of water to surfactant ratio. Nanoparticles of LCMO, NCMO and SCMO were synthesized using the reverse micelle method. In reverse micelle synthesis method reaction time, surfactant chain length plays an important role in controlling the size and shape of the nanoparticles. So, by making use of different chain length surfactant and cosurfactant and reducing the reaction time we find that nanoparticles of narrow size distribution are obtained.

Further the effect of size reduction on electron doped charge ordered manganite $Sm_{0.42}Ca_{0.58}MnO_3$ is investigated by preparing the nanoparticles of average diameter 15 nm, 12 nm, 9 nm and 8 nm by reverse micelle method and compared their properties with the bulk samples. The SQUID measurement of magnetization curve of bulk sample of $Sm_{0.42}Ca_{0.58}MnO_3$ shows a clear CO peak at temperature 280 K. As the size of the nano particles is reduced, the CO transition peak intensity is found to be decreased, broadened and shifted towards the lower temperature, indicating that the CO phase is weakened in the nanosized samples. As the particle size is reduced further to 8 nm, the broad CO peak is found to have completely disappeared. The disappearance of CO is further confirmed by EPR spectroscopy.

A major part of the work also involved the design and development of a Vibrating Magnetometer (VSM) with variable temperature control (100-400 K) measurement capability. It uses a bipolar power supply to energize an electromagnet capable of attaining ±1 Tesla field, subwoofer speaker for vibrating the sample and the induced voltage in four coil setups is measured by a lock-in amplifier. All hardware is controlled by a customized LabView program. The cryostat is designed such that the temperature can be varied continuously from 100K to 400K using liquid nitrogen up to room temperature and forced nitrogen gas/air for high temperatures study. Along with this FORC protocol is implemented using LabView programming which will help to understand magnetic domain state. The VSM sensitivity was validated against commercial systems. This setup help to understand the magnetic phase transition in nanomaterials, offering a cost-effective alternative to commercial magnetometers.

**t0045**

**Studies on ZnO Based Nanogenerators for Vibration Energy Harvesting Applications**

Abhinav Mahapatra[1,2*]
*1Nano-Electronic Materials & Devices Lab., Raja Ramanna Centre for Advanced Technology, Indore-452013, India*
*2 Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400094, India*
**Email: patraabhi007@gmail.com*

With the increasing network of Internet of Things (IoT) networks the demand for sustainable power sources to operate billions of distributed sensors is also increased. Harnessing ambient mechanical vibrations present a promising solution for self-powered systems through piezoelectric nanogenerators (PENGs) and triboelectric nanogenerators (TENGs). In this thesis work, high-performance ZnO-based PENGs and TENGs were developed through material engineering and device architecture optimization. For PENGs, oxygen annealing of ZnO nanostructures reduced oxygen vacancies which lowers free carrier concentration/reduced piezoelectric screening and improved the open-circuit voltage from ~2.5 V to ~5.0 V and the short-circuit current (Isc) from ~4.0 μA to ~6.0 μA. Bulk heterojunction n-ZnO/p-NiO:PDMS PENGs further enhanced output, achieving Voc ~65 V, Isc ~4.1 μA, and ~37.9 μW/cm². ZnO:PVDF PENGs with 10 wt.% ZnO shows Voc ~14.6 V, Isc ~0.6 μA, and ~21.3 μW/cm², showing applications such as a ~99% accurate shoe-insole pedometer and a self-powered UV sensor with 93% sensitivity. For TENGs, MoS2 incorporation into PDMS improved tribonegativity results in fabrication textile integrated single-electrode triboelectric nanogenerator with Voc ~320 V, Isc ~33 μA, and ~3.2 mW/cm² power density, which is capable of biomechanical motion sensing at various bending positions. The performance of final TENG was further improved by Al-doping in ZnO (AZO), inserting a SiO2

interlayer to suppress electron diffusion from AZO to ITO, and using optimized MoS2:PDMS nanocomposite, leads to a final output of Voc ~369 V, Isc ~28.26 μA, and ~1.8 mW/cm² for ZnO-based flexible nanogenerators. These final device powered up to 400 LEDs without any external storage and maintained stable operation over 10,000 cycles and three months. This study provides a systematic approach to enhancing ZnO-based nanogenerator performance, demonstrating practical energy harvesting and sensing capabilities for next-generation self-powered IoT systems.

**t0046**

**Development of Two-dimensional Heterostructures in Energy Storage Device**

Monika Sharma[1, a)] and Pritam Deb[1]

[1] *Advanced Functional Material Laboratory (AFML), Department of Physics, Tezpur University (Central University), Tezpur 784028, India.*

[a)] *Email: monikas@tezu.ernet.in*

In the ever-charging rhythm of the modern world, where energy flows through the core systems of society just like blood through arteries, the call for advanced energy storage grows increasingly urgent. In this regard, supercapacitors and batteries have been widely used. Supercapacitors offer high-power output, prolong cyclability, and quick charge delivery whereas battery provides higher energy density. In this intellectual pursuit, the confluence of materials science and electrochemical ingenuity lies an elegant solution via two-dimensional (2D) materials, layered with purpose and potential to unlock synergies that single materials alone could scarcely summon. The thesis delves into the orchestration of hybrid 2D/2D heterostructures material designed to craft advanced electrodes for storage application. The thesis studies novel 2D based hybrid nanostructures namely $WS_2$@N-rGO, $ZnNi_2O_4/WS_2$, $CuSe/WS_2$, $WS_2/ZnNi_2O_4$, $ZnNi_2O_4/ZnNi_2S_4$, $CuO/ZnNi_2O_4/ZnNi_2S_4$, to fabricate efficient electrodes with enhanced interfacial interactions for supercapacitor and Al-based battery applications. Further, the electrochemical performances of in-plane, out of plane and binder free electrodes are also evaluated. Interestingly, a noteworthy enhancement in electrochemical performance has been observed for $ZnNi_2O_4/ZnNi_2S_4$ hybrid nanostructure under the influence of an external magnetic field, showing promising new phenomenon influencing charge transport and storage behaviour. In addition, the out-of-plane $CuSe/WS_2$, $WS_2/ZnNi_2O_4$ hybrid nanostructures can sustain at differential temperature ranges, depicting their temperature endurability. The real time application of developed systems have been examined using powering 17 red LEDs, green, blue, yellow, scientific calculator, clock and electric motor, highlighting its potential application in next-generation energy storage devices.

**t0047**

**Design and Development of Nanostructured Metal Oxide-Based Hybrid Films for Selective Nitrogen Dioxide ($NO_2$) Detection**

Ankita Pathak [1,2 a)], S. Samanta[1], M. Kaur[1,2], A. Singh[1,2]

[1]*Technical Physics Division, Bhabha Atomic Research Centre, Mumbai-400 085, INDIA*

[2]*Homi Bhabha National Institute, Anushaktinagar, Mumbai-400 085, INDIA*

[a)] *Email: ankitap@barc.gov.in*

Amid escalating pollution and climate concerns, real-time air quality monitoring has emerged as a pressing priority, underscoring the demand for efficient gas sensing devices. The performance of these devices is largely governed by the composition and physicochemical properties of the sensing material. The present work focuses on the rational design and systematic evaluation of nanostructured zinc oxide (ZnO)-based hybrid materials engineered for the efficient detection of $NO_2$ gas. A comprehensive understanding of the governing sensing mechanisms is achieved via coordinated experimental and theoretical investigations. The study identifies ZnO-MgO and $MoS_2$-ZnO hybrids as the most promising systems, owing to their exceptional $NO_2$ sensing performance at room temperature which makes them highly suitable for real-time applications.

**t0048**

**Investigation of Surface Plasmon Resonance in Transition Metal Nitride Thin Films**

Liya Tony and S N Potty*

*(Centre for Materials for Electronics Technology (C-MET)*

*Scientific Society, Ministry of Electronics & Information Technology, Government of India*

*Shoranur Road, Athani P.O, Thrissur 680 581*

**Email: snpotty@cmet.gov.in*

The major objective of the thesis work was to develop transition metal nitride (TMN) thin films (TiN and ZrN) with required carrier concentration to exhibit plasmonic property in the visible region. TMN materials are non-stoichiometric and hence the properties are composition dependent. Here, composition tunablity has been attempted in the films to obtain the targeted properties, by adopting various preparation routes. Sputtering is one of the most widely used physical vapour deposition techniques for coating thin films of transition metal nitrides, and hence this technique was adopted initially. As a novel technique, then opted ammonia nitridation route for the fabrication of plasmonic TiN thin films. Free electrons in a material provide the required negative real permittivity in the frequency of interest, which is an essential property for any plasmonic material. A major disadvantage that needs to be avoided for optimum performance of plasmonic materials is the loss associated with them, arising from the interband electronic transitions, due to the light-matter interaction. For exciting surface plasmons, the evanescent electrical field, generatedat the metal-dielectric interface through a prism geometry, is conventionally adopted for the wavevector matching conditions between incident light and the surface plasmon mode. This process is very much dependent on the thickness of the films. Hence, plasmonic

behavior have been achieved in transition metal nitrides by optimizing the material properties such as carrier concentration and mobility by varying coating parameters, and also by fine-tuning the film thickness.

# y) YOUNG ACHIEVER PAPERS

**y0001**

**Piperazinium Hydrogen Phosphite Monohydrate NLO Single Crystal for Optical Limiting Applications**

R. RAJKUMAR

*Department of Physics SRM Valliammai Engineering College, Kattankulathur – 603 203.*

**Email:rrajkumar2390@gmail.com*

Organic charge transfer molecule of Piperazinium hydrogen phosphite monohydrate single crystal was crystallized by slow evaporation technique. The single crystal XRD was carried out to determine the cell parameter values. The FTIR and FT-Raman spectral studies are used to confirm the presence functional groups. UV-visible spectrum shows that the Piperazinium hydrogen phosphite monohydrate crystal (PHPM) is transparent in the visible region. The third order nonlinear optical refractive index and nonlinear optical absorption coefficient were calculated by Z scan technique. Optical limiting method is applied to find the limiting behavior of Piperazinium hydrogen phosphite monohydrate crystal.

**y0002**

**How Do Quantum Effect Manifest At Ultrathin Flim Limits And What Implications Does This Have For Device Performance?**

Nayan Bhandari

*University of Calcutta, Kolkata , West Bengal*

**Email- nayan.physics@outlook.com*

Quantum Confinement Effect: At ultrathin limits, PdO flims show a clear blue shift in bant gap due to quantization of electronic states from spatial confinement of carriers. Strong alignment between experimental Tauc plots and Hartee- Fock simulations confirms quantum confinement as the driving mechanism. Thikness-dependent band gaps enable precise tuining of device properties, enhancing performance in sensors, photodetectors and catalysts.

Quantum Capacitance Effect: Quantum capacitance arising from changes in DOS varies significantly in ultrathin systems. In TIs, both Zeeman interaction and hybridization modulate magnetocapacitance, revealing beating patterns and SdH oscillation splitting, all of which are essential to charge dynamics and field-effect behavior. Quantum fluctuations in disordered superconductors can significantly affect their transport properties, especially in ultrathin films: In ultrathin superconducting films near the Zeeman-induced quantum critical point, quantum pairing fluctuations driven by virtual quasiparticles cause significant conductivity corrections at zero temperature. These arise from quantized electronic states due to spatial confinement, leading to negative magnetoresistance. This is consistent with enhanced superconductivity observed in amorphous Pb films and oxide interface electron gases under parallel magnetic fields. Collectively, these quantum effects offer powerful mechanisms to engineer and enhance device functionalities at the nanoscale. However, they also demand high-precision fabrication and a deep understanding of quantum-state behavior under external fields and disorder. Exploiting these effects is key to advancing next-generation nanoelectronics, quantum sensors, and superconducting technologies.

**y0004**

**Spin-Projection Fingerprints of Quantized Spin Hall Conductivity in Atomically Thin Topological Materials**

Bahadur Singh[1, *] and Rahul Verma1

*[1]Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Mumbai 400005, India*

**Email: bahadur.singh@tifr.res.in*

Atomically thin two-dimensional topological insulators (2D TIs) protected by time-reversal symmetry can exhibit a quantized spin Hall conductivity (SHC), making them promising candidates for spin-based quantum devices. However, perfect quantization is often hindered by spin mixing due to strong spin-orbit coupling or other material-specific effects. In this work, we discuss a spin-projection feature spectrum as a diagnostic tool for tracking deviations from perfect quantization and identifying the spin quantization axis in real materials. This feature spectrum provides a clear fingerprint that links band topology to spin-resolved properties, guiding the optimal cleaving direction for observing quantized SHC. We validate our approach using materials from our recent studies, including puckered-lattice Sb, which, for the first time, is shown to exhibit double quantum spin Hall effect with SHC ~3.96$e^2$/h enabled by a generic point band inversion and an emergent spin U(1) quasi-symmetry. We also apply this strategy to our bottom-up designed $MoSi_2N_4$-type materials, where symmetry-lowering distortions trigger band inversion and large SHC. Our work provides a unified framework for identifying 2D TIs with robust spin Hall quantization and paves the way toward realizing exotic quantum phases, such as topological superconductivity, efficient spin-charge conversion, and spin-orbit torque phenomena, where spin texture governs phase emergence and properties.

**y0006**

**Crystalline Defects Engineering to Optimize the Thermoelectric Properties of Immiscible Alloys**

Nirmal Kumar Velu*

*CSIR – Institute of Minerals and Materials Technology, Bhubaneswar- 751013, Odisha, India*

**Email: nirmalvelu.immt@csir.res.in*

Thermoelectric (TE) energy conversion is recognized as one of the major green conversion processes to generate electricity because no harmful radiations and emissions are generated during the conversion. Additionally, thermoelectric generators do not contain any moving parts and they convert heat energy in to electrical energy, directly. The major challenge in optimizing a high-performance TE material is their interrelated electrical and thermal conducting properties. Various types of materials with complex

structures and dimensions were analyzed to understand and enhance their TE properties. Nano structuring, multi-grain boundaries, dispersion of an element in bulk materials, alloy formation, structural defects like lattice strains, dislocation and twin boundaries are identified as major strategies to improve the TE performance of materials. We induced various crystalline defects in InGaSb immiscible alloy and studied the role crystalline defects engineering on the electron and phonon transport properties. The thermoelectric figure of merit is enhanced from 0.29 to 0.87, which is thus far one of the best values among any other III-V semiconductors.

**y0007**

**Visualizing Field-induced Solid State Amorphization in 2D Ferroelectric $In_2Se_3$**

Shubham Parathe[1], Gaurav Modi[2], Jishnu Ghosh[1], Vivek Dey[1], Shreyas Agarwal[1], Rishi Jindal[1], Anudeep Tullibilli[1], Arup Basak[1], Ritesh Agarwal[2], Pavan Nukala[1,a]

[1] *Center for Nanoscience and Engineering, IISc Bengaluru, 560012, India*

[2.] *Materials Science and Engineering, LRSM, 3231 Walnut Street, University of Pennsylvania, 19104, USA*

[a)]Corresponding author: pnukala@iisc.ac.in

Part of this paper is published in Nature, **635**, 847–853 (2024), doi: 10.1038/s41586-024-08156-8

Phase change memory suffers reliability issues due to the large power required to write an amorphous phase from crystalline phase via melt-quench mechanism. In this work we show that 2D ferroelectrics can solve this problem by offering a completely field-induced solid-state amorphization pathway, which employs a billion times less power density than the melt-quench pathway. With In2Se3 as a model system, we employ in-situ electron microscopy to directly visualize the structural changes upon applying electrical bias parallel to the van der Waals layers. We find that piezoelectric coupling creates disorder through interlayer sliding, rotation and unravel stress-induced martensitic phase transitions. Interaction between various defects created in these processes results in earthquake-like correlated electromechanical shocks (Barkhausen's noise) that carries the disorder in a longer range, given the weak van der Waals bonds, until eventually the entire length of the device amorphizes. Joule heating switches back the amorphous phase back into the crystalline phase.

**y0008**

**Study of Quantum Spin Chain-Based New Type-II Multiferroics Series with Giant Magneto-Dielectric Coupling**

Sanjay Kumar Upadhyay[1,2*]

[1]*HNB Garhwal University, Srinaagr-Garhwal-246174, Uttarakhand, India.*

[2]*Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai-400005, India*

**Email:skuphysics@gmail.com*

In the present work, first, the discovery of a new type-II multiferroicity in Haldane spin-chain $Tb_2BaNiO_5$ has been discussed in detail. Two antiferromagnetic transitions ($T_1$= 64 K and $T_2$= 25 K) have been obtained for $Tb_2BaNiO_5$, and the lower antiferromagnetic transition, $T_2$= 25 K, also comes out to be ferroelectric, the typical signature of type-II multiferroicity. The second section of the present work will discuss how the discovery of multiferroicity in $Tb_2BaNiO_5$ ultimately led to the identification of an entirely new type-II multiferroic series, $R_2BaCoO_5$ (R = Tb, Sm). $Tb_2BaCoO_5$ shares both (antiferromagnetic and ferroelectric) transitions at 19 K and it shows the largest magneto-dielectric coupling (e.g., close to 55%) among all polycrystalline type-II multiferroics. While $Sm_2BaCoO_5$ exhibits both antiferromagnetic and ferroelectric transitions at 38 K. Therefore, the experimental results presented in the present work show that we have identified $R_2BaCoO_5$ (R = Tb, Sm) — spin-chain–based cobaltates — as a new, previously unexplored multiferroic series.

**y0009**

**Investigation of Optical Transitions and Band Gap in Layered $MoS_2$ using UV Spectroscopy**

Amodini Mishra[1 a)*]

[1]*Indian Institute of Technology Delhi, Hauz Khas, New Delhi 110016, India)*

[a)*]Email: amodiniphysics@gmail.com

In this work, we report the synthesis of layered $MoS_2$ using a one-step hydrothermal method. Raman spectroscopy reveals two prominent peaks corresponding to the in-plane ($E_2g^1$) and out-of-plane ($A_1g$) vibrational modes, confirming the layered structure of the material. The X-ray diffraction (XRD) pattern indicates the polycrystalline nature of the synthesized $MoS_2$, while atomic force microscopy (AFM) analysis confirms the low surface roughness. Optical absorption spectra obtained from UV–Vis measurements suggest an indirect band gap transition with an estimated band gap energy of approximately 1.4 eV. This study highlights the potential of layered $MoS_2$ for application in next-generation optoelectronic devices.

**y0010**

**Spin–Phonon Coupling and Optoelectronic Property Studies in RE-Doped $Bi_4Ti_2(Fe/Co)O_{12}$ Aurivillius Ceramics**

Patri Tirupathi[a], S. Rayaprol[b], and P.D. Babu[b],

[a]*University Department of Physics, Tilka Manjhi Bhagalpur University, Bhagalpur-Bihar -812007- India*

[b]*UGC-DAE Consortium for Scientific Research, Mumbai Center, BARC, Mumbai - 400085, India*

[a)] Corresponding author: *ptirupathi36@gmail.com*

Rare earth ion-doped multiferroic $Bi_{3.0}RE_{1.0}Ti_2(Fe_{0.5}Co_{0.5})O_{12}$ n=3 layered Aurivillius ceramics were synthesized using the conventional solid-state reaction method. The X-ray diffraction study confirms the phase purity and crystal structure of the Aurivillius ceramics as orthorhombic with a B2cb space group. The spin-phonon coupling by Raman study supports the layered structure formation. The photoluminescence study confirms the f-f & f-d band emissions, and tuning of band gap energy calculations. The P-E energy density study was investigated to assess optoelectronic device applications.

**y0011**

**SCAPS Simulation of Lead-Free Cs2AuBiCl6 Double Perovskite-Based Solar Cell**

Arpana Agrawal* and Shramank Chaturvedi

*Department of Physics, Prime Minister College of Excellence, Shri Neelkantheshwar Government Post-Graduate College, Khandwa-450001, India*

**Email: agrawal.arpana01@gmail.com (Email of corresponding author)*

This study investigates the response of $Cs_2AuBiCl_6$/$CuSbS_2$-based solar cell structure using SCAPS simulation. $Cs_2AuBiCl_6$ perovskite is more stable than Sn, Cu, Ti, and Pb-based perovskite, and environmentally friendly. $Cs_2AuBiCl_6$ material exhibits a high absorption coefficient of approximately $10^5$ $cm^{-1}$, accompanied by low reflectance and an energy band gap of 1.12 eV, enabling it to absorb light with longer wavelengths, making it an optimal absorber material. The key performance parameters, i.e., short-circuit current density ($J_{sc}$), open-circuit voltage ($V_{oc}$), fill factor (FF), and power conversion efficiency (PCE), have been evaluated using various experimentally reported parameters. The influence of absorber layer parameters, including thickness, energy band gap, electron affinity, and doping concentration, on solar cell performance has been assessed. The simulated performance parameters $V_{OC}$, $J_{SC}$, FF, & PCE are 1.14 V, 34.25 mA/cm², 89.05%, and 34.71%, respectively, for an optimized solar cell, suggesting its utility for efficient solar cells.

**y0013**

**Wearable Humidity Sensors For Human Healthcare Applications**

Komal Bapna[1,2, a)], Parvesh Kumari[1,2], Ankit Solanki[1,2], G. Gupta[1] and D. D. Shivagan[1,2]

*[1]CSIR- National Physical Laboratory, Dr. K. S. Krishnan Marg, New Delhi 110 012, India*

*[2]Academy of Scientific and Innovative Research (AcSIR), Ghaziabad- 201 002, India*

*[a)]Email: komal.nplindia@csir.res.in*

SI traceable GO, GO-Chitosan and GO-Cellulose based physio-resistive type humidity sensors have been developed and studied for their humidity sensing characteristics, such as, response-recovery, long term stability, repeatability, selectivity, etc. We have demonstrated the applications of these humidity sensors for real time respiratory, skin moisture monitoring and apnea like situations along with their ability to recognize speech pattern. The paper discusses the simple, cost-effective synthesis process and physio-resistive properties of these sensors which make them a viable solution to be utilized in wearable human healthcare and human interactive advanced technologies.

**y0014**

**Microwave Dielectric Properties of Ca-doped $Sr_2SnO_4$ Ceramics with Ruddlesden–Popper Structure for Communication Applications**

Upendra Kumar

*Advanced Functional Materials Laboratory, Department of Applied Sciences, IIIT Allahabad, Prayagraj-211015, U.P., India*

*Email: upendrakumar@iiita.ac.in; Tel:+91-532-292-2525*

This study reports the synthesis and microwave dielectric characterization of $(Sr_{1-x}Ca_x)_2SnO_4$ ceramics (x = 0–0.06), prepared via a conventional solid-state reaction. All compositions crystallized in the tetragonal Ruddlesden–Popper (R-P) structure with space group I4/mmm. Systematic reduction in lattice parameters with increasing $Ca^{2+}$ concentration confirmed successful substitution at the A-site. FTIR and Raman spectroscopy confirmed the structural integrity of the R-P phase, with characteristic vibrational bands appearing near 726, 582, and 570 $cm^{-1}$. Dielectric measurements revealed notable enhancement in the relative permittivity ($\varepsilon_r$) and quality factor (Q×f), peaking at x = 0.02, along with a substantial reduction in the temperature coefficient of resonant frequency ($\tau_f$). The optimal composition, x = 0.02, exhibited $\varepsilon_r \approx 33$, Q×f ≈ 32,517 GHz, and $\tau_f \approx 1.45$ ppm/°C, suggesting promising applicability in next-generation microwave communication systems.

**y0015**

**Microscopic evidence of field-induced critical spin-liquid state in a metallic frustrated compound**

I. Ishant,[1] K. Bhattacharya,[1] R. Scheuermann,[2] Z. Guguchia,[2] V. Fritsch,[3] O. Stockert,[4] and M. Majumder[1, *]

[1]*Department of Physics, Shiv Nadar Institution of Eminence, Gautam Buddha Nagar, Uttar Pradesh 201314, India*

[2]*Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland*

[3]*Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany*

[4]*Max Planck Institute for Chemical Physics of Solids, Dresden, Germany*

A field-induced quantum spin liquid (QSL) state is an extraordinary phenomenon, hitherto unobserved in metallic frustrated compounds. CePdAl, a magnetically frustrated metallic compound with a kagome lattice, presents a unique opportunity to explore this phenomenon [1]. Recent bulk measurements have revealed intriguing magnetic states in CePdAl when a magnetic field is applied along the crystallographic c-axis [2]. However, the nature of these field-induced states, potentially including a QSL state, remains unclear due to the lack of microscopic investigation. To elucidate these field-induced states, we employed the transverse-field muon spin relaxation/rotation (TF-μSR) technique, applying various magnetic fields parallel to the c-axis in single-crystalline CePdAl over a broad temperature range (100 K-100 mK). Our findings indicate that field-induced low-temperature states for fields B≤ Bc2 exhibit long-range magnetic order, whereas for B>Bc2 yield contrasting behavior. Notably, at 3.75 T, near a critical field Bc2, our results provide evidence of a critical spin liquid (CSL) with antiferromagnetic spin fluctuations. Furthermore, at 4.3 T, a non-Fermi liquid state is observed where frustration is absent. This comprehensive microscopic study unequivocally establishes the existence of a CSL state in a metallic frustrated system, for the first time to the best of our knowledge.

**y0016**

**Active gamma shielding design for Hard Xray detector in Aditya-U.**

Samridhi[1]*, Shishir Purohit[2], and Manoj Kumar Gupta[2]
*1 Institute for Plasma Research (IPR), Bhat P.O. Gandhinagar, Gujarat, 382428.*
*2 Homi Bhabha National Institute, Training School Complex, Anushaktinagar, Mumbai, 400094, India.*
*Corresponding author*: samridhi@ipr.res.in*

In Aditya-U tokamak, hard X-rays (HX) generated by runaway electrons via bremsstrahlung interactions are typically detected using high-density scintillation detectors like $LaBr_3$(Ce). These detectors convert high-energy photon interactions into electrical signals, enabling spectral and intensity diagnostics. Currently, lead-based shielding is employed to protect detectors[1]; however, lead suffers from poor mechanical strength, potential structural degradation, and significant environmental concerns, necessitating periodic safety assessments.

Given the isotropic nature and high flux of HX radiation in tokamaks, shielding must ensure unidirectional photon entry to maximize signal-to-noise ratio and prevent detector pile-up. In this work, we investigate alternative shielding strategies—including both single-material and multilayer designs—to improve upon the limitations of lead (Pb)[2,3]. Materials are evaluated based on attenuation efficiency for photons >100 keV, structural robustness, and suitability for integration into the diagnostic environment of Aditya-U[4]. The optimized shielding and collimation configurations aim to enhance detection accuracy, directionality, and long-term reliability for HX diagnostics in fusion plasmas.

**y0017**

**Substrate Dependent Growth Study of $ZnIn_2S_4$ Nanostructures: Single Step Hydrothermal Approach**

Prashant K. Bankar
*Centre for Advanced Studies in Materials Science and Condensed Matter Physics, Department of Physics, Savitribai Phule Pune University, Pune – 411 007, India*
**Email:bankarprashant26@gmail.com*

The unique structural features and fascinating physicochemical properties of 2D nanostructured materials have shown great application in charge storage, optoelectronics and photoconduction device. Zinc Indium Sulfide (ZnIn2S4) is the only member of the ternary metal sulfides family with a layered structure. Amongst the methods used for synthesizing ZnIn2S4 structures, the hydrothermal technique offers a simple, cost-effective and environmentally friendly route for materials synthesis. To study the effect of substrate on the formation of hydrothermally grown ZnIn2S4 on several types of substrates were used. The structures of the ZnIn2S4 were systematically studied by scanning electron microscopy (SEM) and XRD. It was demonstrated that the type of substrates used had a great influence on the morphologies, density and alignment of the ZnIn2S4 formed. The ordered structure of nanometric dense ZnIn2S4 has been prepared on the conductive substrate for practical application in nano electronic devices.

**y0018**

**Comparative Analysis of Spectroscopic and Laser Characteristics of Nd doped Vanadate Single Crystals**

M. Soharab[*1], R. Bhatt[1,2], N.S. Benerji[1] and Indranil Bhaumik[#1,2]
*[1]Crystal Growth Laboratory & Laser Materials Instrumentation Laboratory, High Energy Lasers & Optics Division*
*Raja Ramanna Centre for Advanced Technology, Indore-452 013, India*
*[2]Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai-400 094, India*
*Corresponding authors: *sohrab@rrcat.gov.in; [#]neel@rrcat.gov.in*

Single crystals of Nd doped vanadates (namely $YVO_4$, $GdVO_4$ and $LuVO_4$), a family of important laser gain medium for compact solid-state laser, were grown by optical floating zone technique. A comparative spectroscopic investigation based on Judd-Ofelt theory revealed that the spectroscopic quality factor and product of radiative lifetime as well as emission cross-section are the best for Nd:$GdVO_4$ crystal. In line with the observation, the Nd:$GdVO_4$ exhibits the best lasing performance as well. Further, after anti-reflection coating, near Gaussian beam ($M^2$ ~2.6) with output power ~14 W and slope efficiency ~53% was achieved in the element fabricated from the grown Nd:$GdVO_4$ crystal.

**y0019**

**Unity of universal parameter α in an overdoped single crystal of high temperature superconductor $Bi2Sr2CaCuO_{8+\alpha}$**

Gourav Vaid[1]

[1] *School of Physics, Indian Institute of Science Education and Research, Thiruvananthapuram 695551, India*

*Email: vaidgourav21@iisertvm.ac.in*

Recently, it has been observed that in some high temperature superconductors such as LSCO and Bi-2201, the temperature dependence of resistivity is found to be linear [1]. Such a linear temperature dependence of resistivity is assumed to arise due to a linear drop of quasiparticle decay rate Γ with temperature enabling the existence of a Planckian dissipation timescale $\tau \equiv \hbar/\Gamma$ in the system in overdoped samples[2]. In this work, we present the temperature dependence of resistivity in highly pure single crystals of $Bi_2Sr_2CaCuO_{8+\delta}$ (BSCCO-2212) that were grown using a pressure technique and have been found to have minimal amount of intergrowth of competing BSCCO-2201 phase. By doing a linear fit to the temperature dependence of resistivity in the normal state, we were able to obtain the value of the universal parameter (α), given by the relation $h/\tau = \alpha k_B T$.

**y0020**

**Large Magnetocaloric Effect and Dual Magnetic Transitions in GdRhIn**

A. A. Maz, R. Kumar and S. Gupta

*Department of Physics, Bennett University, Greater Noida – 201310, India*

**Corresponding author: [e23soep0034@bennett.edu.in]*

We present detailed insights into structural, magnetism and magnetocaloric properties of the RTX-type inter- metallic GdRhIn. Using room-temperature X-ray diffraction showed the hexagonal Fe2P-type structure (space group $P\bar{6}2m$). Magnetization data reveals antiferromagnetic order below TN = 16 K then after it showed ferromagnetic transition till TC = 34 K, and the after it showed paramagnetic characteristics. The isothermal magnetic-entropy change reaches ΔSM =10.3 J kg−1 K−1 for the applied field 70 kOe, while the relative cooling capacity RC = 282 J kg−1 for 50 kOe. The large magnetocaloric effect and tunable transition temperatures render GdRhIn a promising candidate for low-temperature magnetic refrigeration and cryogenic sensing.

**y0021**

**Oxygen-Free Fabrication Unlocks High-Mobility Transport and Quantum Dot Control in van der Waals Heterostructures**

Subhrajit Mukherjee,[1,2,a)] Dasari Venkatakrishnarao,[2] Sarthak Das,[2] Ivan A. Verzhbitskiy,[2] Yee Sin Ang,[3] Kuan Eng Johnson Goh[2,4] and Chit Siong Lau[2,3]

[1] *Department of Physics, School of Natural Sciences, Shiv Nadar Institution of Eminence, Delhi-NCR, Gautam Buddha Nagar, Uttar Pradesh, India 201314*

[2] *Quantum Innovation Centre (Q.InC), Agency for Science Technology and Research (A*STAR), Singapore 138634.*

[3] *Science, Mathematics and Technology, Singapore University of Technology and Design, Singapore 487372.*

[4] *Department of Physics, National University of Singapore, Singapore 117551.*

[a)] *Corresponding author: Subhrajit.mukherjee@snu.edu.in*

Two-dimensional transition metal dichalcogenides promise exceptional performance in nanoelectronic and quantum devices but often fall short due to extrinsic disorder introduced during fabrication. Here, we demonstrate the ambient oxygen exposure during lithographic processing as a dominant, yet underappreciated source of charge doping and mobility degradation, even for nominally "ambient-stable" TMDs. By implementing an entirely oxygen-free device fabrication protocol inside an inert glovebox, we achieve monolayer MoS2 and WS2 field-effect transistors with mobilities approaching theoretical phonon-limited values and reduced variability across large device arrays. Density functional theory (DFT) reveal that O2 rapidly chemisorbs on defect sites, creating deep traps that persist despite mild annealing. Beyond performance recovery, our oxygen-free process enables ultraclean van der Waals heterostructures suitable for low-disorder quantum devices. We demonstrate gate-defined quantum dots in WS2 heterostructures, achieving single-electron transport at 43 mK. This work establishes oxygen-free fabrication as a straightforward and broadly applicable route to intrinsic-limit transport and quantum-ready 2D devices.

**y0022**

**DFT Investigation on the Structural, Electronic and Optical Properties of $SmVO_4$ Orthovanadates**

Rachana Sain[1,*] and Chandan Upadhyay[1]

[1] *School of Materials Science and Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi, UP-221005, India.*

**Email: rachanasain.rs.mst20@iitbhu.ac.in*

We present an integrative first-principles study of zircon-type samarium orthovanadate, $SmVO_4$, unifying structural optimization, electronic band structure, density of states (DOS), joint density of states (JDOS), dielectric response, and electron energy loss spectra (EELS) into a single, quantitative framework. The optimized lattice constants, a = 7.289 Å, c = 6.385 Å closely match experiments and confirming the stability. A direct band gap of 2.89 eV is identified, with O–2p and V–3d states dominating the valence and conduction bands, respectively, and notable Sm–4f hybridization. The static dielectric constant $\varepsilon_1(0) = 4.62$ and the $\varepsilon_2(\omega)$ peak at 5.3 eV highlight strong O–2p → V–3d optical transitions. Low loss EELS interpretation captures plasmonic and inter band transitions, directly matching with JDOS spectral peaks. This study uniquely resolves the structural, electronic, optical, and

EELS–JDOS correlations, setting a benchmark methodology for probing rare-earth orthovanadates and advancing their application in UV–Vis optoelectronics.